

Programming Environment and Training Annual Report - Year Three

Programming Environment and Training Annual Report - Year Three July 1999

Work funded by the DoD High Performance Computing Modernization Program CEWES Major Shared Resource Center

Produced in support of Contract Number: DAHC 94-96-C002 by Nichols Research

Views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of Defense position, policy, or decision unless so designated by other official documentation.

Approved for public release, distribution is unlimited.

This page intentionally left blank

Table of Contents

Εx	ecutive Summary	XIII
1.	INTRODUCTION	I-1
	1.1 The DoD High Performance Computing Modernization Program (HPCMP)	1-1
2.	CEWES MSRC PET STRATEGIC PLAN	2-1
	2.1 Goals and Objectives	2-1
	2.2 Approach	2-2
	2.3 Core Support	2-3
	2.4 Focused Efforts	2-3
	2.5 Training	2-4
	2.6 Outreach	2-4
	2.7 HBCU/MI Program	2-4
3.	IMPLEMENTATION	3-1
	3.1 Management	3-1
	3.2 Organization	3-1
	3.3 Team Composition	3-1
	3.4 Reporting and Technology Transfer	3-3
4.	TECHNICAL SUPPORT TEAMS	1-1
	4.1 CFD: Computational Fluid Dynamics CTA (ERC – Mississippi State)	4-2
	4.2 CSM: Computational Structural Mechanics CTA (TICAM - Texas, with ERC - Mississippi State)	4-2
	4.3 CWO: Climate/Weather/Ocean Modeling and Simulation CTA (Ohio State)	4-3
	4.4 EQM: Environmental Quality Modeling and Simulation CTA (TICAM - Texas)	4-4
	4.5 FMS: Forces Modeling and Simulation/C4I CTA (NPAC - Syracuse)	4-4
	4.6 C/C: Collaboration and Communications (NPAC - Syracuse	4-4

4	I.7 SPP Tools: Scalable Parallel Programming Tools (CRPC – Rice and ICL - Tennessee	4-5
4	I.8 SV: Scientific Visualization (NCSA - Illinois, with ERC - Mississippi State)	4-6
5. YE	EAR 3 MAJOR ACCOMPLISHMENTS	5-1
5	5.1 CFD: Computational Fluid Dynamics CTA (ERC - Mississippi State)	5-1
	5.1.1 Parallel CGWAVE	5-1
	5.1.2 Parallel CH3D/SED	5-2
5	5.2 CSM: Computational Structural Mechanics CTA (TICAM - Texas, with ERC - Mississippi State)	5-3
	5.2.1 CTH: Block Adaptive Strategy	5-4
	5.2.2 EPIC: Simplex Refinement Strategy	5-5
5	5.3 CWO: Climate/Weather/Ocean Modeling CTA (Ohio State)	5-5
	5.3.1 Integrated Coastal Modeling Systems (ICOMS)	5-6
5	5.4 EQM: Environmental Quality Modeling CTA (TICAM - Texas)	5-7
	5.4.1 Parallel CE-QUAL-ICM	5-7
	5.4.2 Parallel ADCIRC	5-7
	5.4.3 Coupling ADCIRC and CE-QUAL-ICM: Projection –UTPROJ	5-8
	5.4.4 Transport Schemes on Unstructured Meshes: CE-QUAL-ICM	5-9
	5.4.5 Web Launching: PARSSIM	5-9
5	5.5 FMS: Forces Modeling and Simulation/C4I CTA (NPAC - Syracuse)	5-10
	5.5.1 WebHLA Activities	5-10
	5.5.2 WebFlow Activities	5-13
5	5.6 C/C: Collaboration and Communications (NPAC - Syracuse)	5-14
	5.6.1 TANGO Interactive: Distance Training and Collaboration	5-15
5	5.7 SPP Tools: Scalable Parallel Programming Tools (CRPC – Rice and ICL - Tennessee)	5-16
	5.7.1 HELIX: Scalar Optimization (Rice)	5-17
	5.7.2 HELIX: OpenMP (Rice)	5-18
	5.7.3 CAPTools (Rice)	5-18
	5.7.4 Web-based SPP Tools Repository (Tennessee)	5-18
	5.7.5 CGWAVE: MPI_Connect (Tennessee)	5-19

	5.7.6 Virtual Reality Immersion for Performance Analysis: Virtue and Vampir (Tennessee)
	5.8 SV: Scientific Visualization (NCSA - Illinois, with ERC - Mississippi State)
	5.8.1 CbayVisGen and CbayTransport (NCSA): EQM 5-2
	5.8.2 DIVA and ISTV (MSU): CWO
	5.8.3 volDG (MSU): CSM
	5.8.4 Computational Monitoring and Interactive Steering (NCSA): EQM 5-22
	5.9 USC HPC Benchmarking
6.	TOOLS INTRODUCED into CEWES MSRC 6-1
	6.1 Programming Tools
	6.1.1 TotalView
	6.1.2 Vampir
	6.1.3 MPI_Connect
	6.1.4 Virtue
	6.1.5 PAPI
	6.1.6 dyninst
	6.1.7 DPCL
	6.1.8 Repository in a Box (RIB)
	6.1.9 CAPTools
	6.2 Previously-Evaluated Tools
	6.2.1 nupshot
	6.2.2 AIMS
	6.2.3 SvPablo
	6.2.4 ParaDyn
	6.2.5 MPE Graphics Library
	6.2.6 ScaLAPACK
	6.2.7 PETSc
	6.3 Visualization Tools
	6.3.1 CbayVisGen and CbayTransport
	6.3.2 Collaborative Data Analysis Toolsuite (CDAT) 6-8

	6.3.3 volDG
	6.3.4 ISTV
	6.4 Communication/Collaboration Tools 6-9
	6.4.1 TANGO Interactive
	6.5 Computational Tools
	6.5.1 WebHLA
	6.5.2 CTH and EPIC Tools
	6.5.3 Integrated Memory Hierarchy (IMH) Model 6-11
7.	USER TRAINING
	7.1 Training Curriculum
	7.2 Training at the DoD HPCMP User Group Meeting
	7.3 Seminars
	7.4 Web-Based Training
	7.5 Training Course Descriptions
	7.5.1 Parallel Programming Workshop for Fortran Programmers
	7.5.2 Using the Message Passing Interface (MPI) Standard 7-3
	7.5.3 Large Deformation Computational Structural Mechanics Applications on High Performance Computers using ParaDyn/DYNA3D
	7.5.4 Grid Generation for Complex Configurations
	7.5.5 Java for Scientific Computing
	7.5.6 High Performance Fortran (HPF) in Practice
	7.5.7 Performance Optimization
	7.5.8 Topics in Finite Element Methodology for Nonlinear Problems 7-5
	7.5.9 A Tutorial on Designing and Building Parallel Programs
	7.5.10 An Introduction to the Fortran 90
	7.5.11 Scalable OpenMP Programming on Origin2000 7-6
	7.5.12 TANGO for Remote Consulting
	7.5.13 Parallel Debugging and Performance Analysis Tools: TotalView and Vampir
	7.5.14 Techniques in Code Parallelization
	7.5.15 Parallel Programming on the SGI/CRAY Origin2000 using OpenMP 7-7

	7.5.16 Computational Monitoring Using CUMULVS	}
	7.5.17 Interactive Structured Time-varying Visualizer (ISTV)	}
	7.5.18 WebFlow: Web Interfaces for Computational Modules	}
8.	SUPPORT of CEWES MSRC USERS	
	8.1 CFD: Computational Fluid Dynamics CTA (ERC -Mississippi State)	
	8.2 CSM: Computational Structural Mechanics CTA (TICAM - Texas, with ERC - Mississippi State) 8-2	<u>)</u>
	8.3 CWO: Climate/Weather/Ocean Modeling and Simulation CTA (Ohio State)	}
	8.4 EQM: Environmental Quality Modeling and Simulation CTA (TICAM - Texas)	ļ
	8.5 FMC: Forces Modeling and Simulation/C4I CTA (NPAC - Syracuse) 8-5	,
	8.6 C/C: Collaboration and Communications (NPAC - Syracuse) 8-6	;
	8.7 SPP Tools: Scalable Parallel Programming Tools (CRPC - Rice, Tennessee)	j
	8.8 SV: Scientific Visualization (NCSA - Illinois, with ERC - Mississippi State))
	8.9 University of Southern California)
	8.10 Clark Atlanta	
9.	HBCU/MI ENHANCEMENT PROGRAM	
	9.1 PET Team at Jackson State	
	9.2 PET Team at Clark Atlanta) -
	9.3 Jackson State HPC Summer Institute)
	9.4 Jackson State Distance Learning	;
	9.5 Jackson State PET Technical Support	}
	9.6 Clark Atlanta PET Technical Support	}
10.	CEWES MSRC/PET TECHNICAL REPORTS 10-1	

This page intentionally left blank

List of Figures

Figure 5-1. CEWES MSRC HPC Challenge Team at SC98 in Orlando
Figure 5-2. Model of fluid flow with sediment transport 5-2
Figure 5-3. Adaptive CTH simulation of copper ball impacting a steel plate
Figure 5-4. EPIC simulation of a rod penetrating a plate 5-5
Figure 5-5. Number of processors and speedup for parallel ADCIRC computations on Cray T3E
Figure 5-6. GUI for launching the simulation code PARSSIM 5-9
Figure 5-7. Integration of commodity web technology for distributed objects with DMSO/RTI
Figure 5-8. Mak Stealth visualization for parallel CMS simulation of a heavy breach operation through a minefield in the Fort Knox terrain
Figure 5-9. WebFlow Java client interface to access remote resources 5-13
Figure 5-10. Remote users participating in a Tango training class taught at the CEWES MSRC
Figure 5-11. Sites linked by MPI_Connect during the SC98HPC Challenge computation
Figure 5-12 WAM visualization of the El Nino event in the Pacific Basin . 5-22
Figure 6-1. Evaluation of performance and debugging tools 6-7
Figure 6-2. Visualization of dissolved oxygen in Chesapeake Bay 6-8
Figure 6-3. Model for the analysis of algorithms and code performance on HPC platforms
Figure 7-1. MSU transmission equipment used in the satellite broadcast of the first HPCMP MSRC training class (1996) 7-1

This page intentionally left blank

List of Tables

Table 1 TECHNICAL SUPPORT TEAM PERSONNEL
Table 2 TEAM TRAVEL
Table 3 CEWES USER CONTACTS
Table 4 TOOLS IMPLEMENTED
Table 5 CEWES MSRC USER CODES IMPACTED
Table 6 TECHNOLOGY TRANSFER
Table 7 TRAINING COURSES
Table 8 TRAINING COURSES & SEMINARS at HBCU/MIs
Table 9 HBCU/MI STUDENTS IMPACTED
Table 10 JOURNAL PAPERS and CONFERENCE PRESENTATIONS 20-

This page intentionally left blank

EXECUTIVE SUMMARY

The true deliverable of the CEWES MSRC Programming Environment and Training (PET) effort is the raised level of CEWES MSRC user capability and programming environment in the CEWES MSRC – to a level not surpassed by academic, industry, or other government HPC centers. The CEWES MSRC PET team addresses this charge by providing core support to CEWES MSRC users, performing specific focused efforts designed to introduce new tools and computational technology into the CEWES MSRC, conducting training courses and workshops for CEWES MSRC users, and operating an HBCU/MI enhancement program. This report covers the CEWES MSRC PET contract year 3 activities from 27 March 1998 through 26 March 1999.

The PET team had a number of successes in Year 3. Team member Rice University hosted the 1998 DoD HPCMP Users Group Meeting for the CEWES MSRC. The PET team offered five training classes, which were very well received. CDROMs containing PET Technical Reports and training material were also produced and distributed at the Users Group Meeting. Expanded efforts in distance learning resulted in college credit courses of study at HBCUs Jackson State, Morgan State, and Clark Atlanta. PET training classes held at the CEWES MSRC went out over the web to users at NRL, ARL, and ASC. The CEWES MSRC PET team supported and participated in the HPC Challenge Team at SC98. That award-winning effort increased the visibility of the CEWES MSRC and the entire HPC modernization program. Syracuse successfully conducted a metacomputing experiment at SC98 with the Computational Mine Simulation program running at the CEWES and ARL MSRCs. The objective was to simulate actual battlefield conditions.

The PET component of the DoD HPC MSRCs is a bold and innovative university/industry/government effort to provide the essential user support and mode of capability enhancement that is necessary for the MSRCs to reach a level comparable to that in the foremost university, industry, and other Government agency HPC centers – and to address the wide variety of research and development demands arising from the science and technology programs supporting DoD's weapons development and warfighting support systems. The purpose of the PET component of the MSRCs is to enhance the entire programming environment for the MSRC users through training and support for software enhancement, addressing both near—term improvements and long—term expansions, thus enabling use of the MSRC computing resources to fullest capacity and extending the range of applicability of HPC to DoD technical problems.

The PET effort is unprecedented in its concept and vision, in its management for long-term achievement, in its strong university commitment, in its approach through unique university/DoD collaboration, in its understanding and relationship between university researchers and MSRC users – and in its challenge to be faced in the interest of DoD by the universities and companies involved, the MSRC users, and the program management. The PET component of the MSRC program is thus a true intellectual enterprise which breaks new ground in collaborative effort between DoD and academia in order to establish a two–way conduit of information and expertise enhancing the capability of the MSRC user and bringing demands of DoD HPC to bear early–on in programming environment developments in progress in the universities.

The CEWES MSRC PET effort is administered by the prime contractor, Nichols Research Corporation (NRC), as a part of the contract for the CEWES MSRC. Mr. Ray Burgess is Acting PET Director. Prof. Joe Thompson of Mississippi State University is CEWES MSRC PET academic team leader. Dr. Wayne Mastin of Nichols, and a professor emeritus of Mississippi State, is the on–site PET team leader. Prof. Willie Brown of Jackson State University is the HBCU/MI leader. Dr. Louis Turcotte of the CEWES MSRC excercises oversight of the CEWES MSRC PET effort for the government.

The fundamental mode of operation for PET at the CEWES MSRC is a direct and continual connection between the CEWES MSRC users and the CEWES MSRC PET team universities in support of the five Computational Technology Areas (CTAs) supported at the CEWES MSRC and three related technical infrastructure areas. This is accomplished through a combination of full—time university and NRC personnel on—site at the CEWES MSRC, in close communication with completely dedicated university personnel dividing time between the CEWES MSRC and the university, and with faculty members at the university with partial time commitment to the CEWES MSRC PET effort for support and leadership.

The university PET team for the CEWES MSRC is led by the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, with Jackson State University as the lead HBCU/MI. The university team is as follows:

- Engineering Research Center for Computational Field Simulation (ERC) at Mississippi State University (NSF Engineering Research Center at Mississippi State)
- Jackson State University

- National Center for Supercomputing Applications (NCSA) at University of Illinois (NSF PACI Center at Illinois)
- Center for Research in Parallel Computing (CRPC) at Rice (NSF Science and Technology Center headquartered at Rice)
- Innovative Computing Laboratories (ICL) at University of Tennessee, Knoxville
- Northeast Parallel Architectures Center (NPAC) at Syracuse University
- Ohio Supercomputer Center (OSC)
- Ohio State University
- Texas Institute for Computational and Applied Mathematics (TICAM) at University of Texas, Austin
- University of Southern California
- Clark Atlanta University

Dedicated on–site/at–university support teams for each of the five DoD Computational Technology Areas (CTAs) supported at the CEWES MSRC were the responsibility of specific universities on the PET team at the CEWES MSRC in Year 3:

- CFD: Computational Fluid Dynamics ERC (Mississippi State)
- CSM: Computational Structural Mechanics TICAM (Texas) and ERC (Mississippi State)
- CWO: Climate/Weather/Ocean Modeling and Simulation Ohio State
- EQM: Environmental Quality Modeling and Simulation TICAM (Texas)
- FMS: Forces Modeling and Simulation / C4I NPAC (Syracuse)

as were each of the following three technical infrastructure support areas:

- Scalable Parallel Programming Tools CRPC (Rice) and ICL (Tennessee)
- Scientific Visualization NCSA (Illinois)
- Collaboration/Communication NPAC (Syracuse)

During Year 3 Mississippi State, Texas, Ohio State and Rice maintained on—site university personnel at the CEWES MSRC in support of CFD (Dr. Steve Bova – MSU), CSM (Dr. Rick Weed – MSU), EQM (Dr. Phu Luong – Texas) and Scalable Parallel Programming Tools (Dr. Clay Breshears – Rice). NCSA at Illinois had a dedicated person spending significant time on—site in support of Scientific Visualization (Dr. Alan Shih) and Ohio State had a dedicated person spending significant time on—site in support of CWO (Dr. David Welsh). NRC had a person on—site in support of Scientific Visualization (Dr. Richard Strelitz – SAIC) and also had a Training Coordinator (John Eberle – NRC) on—site.

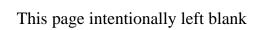
Since the great majority of users of the CEWES MSRC are off-site, the PET effort at the CEWES MSRC places emphasis on outreach to remote users through visits to major remote user sites, training courses at such remote sites, web-based remote training delivery, and remote communication via email and the CEWES MSRC PET website.

During Year 3, the CEWES MSRC PET team included 115 people from 10 universities. The team made direct contact with 61 CEWES MSRC users at 12 sites, and had 318 person—days on—site at CEWES MSRC in addition to the permanent on—site members. There were 19 person—days of travel to conduct remote training for CEWES MSRC users, and 214 person—days of travel to meetings and workshops directly related to the CEWES MSRC PET effort. And there were 239 person—days of travel to national meetings for presentations related to the CEWES MSRC PET effort, to meet CEWES MSRC users, and to track technology developments in the interest of the CEWES MSRC

PET effort. The CEWES MSRC PET team had direct impact on 24 codes in use at CEWES MSRC and introduced 17 programming, computational, visualization, and collaboration tools into CEWES MSRC. The CEWES MSRC PET team carried out 31 specific Focused Efforts during Year 3 to enhance the programming environment at the CEWES MSRC. The team logged 44 person-days at remote sites and 36 person-days at Jackson State.

A total of 17 training courses covering 37 days were conducted on—site at CEWES MSRC, and 8 courses covering 15 days were conducted at 3 remote sites. These training courses were attended by 81 CEWES MSRC users from CEWES and 91 from other CEWES MSRC user sites. A Specialty Workshop on Adaptive Grids was conducted, with nine presentations, including two from CEWES MSRC users. The HPC Summer Institute was conducted at Jackson State and attended by 20 students from HBCUs. Three regular semester courses were conducted at Jackson State over the web, as well as one at Clark Atlanta and one at Morgan State, impacting 46 students from these HBCUs. The CEWES MSRC PET team

produced 41 CEWES MSRC/PET technical reports, 29 conference presentations, and 6 journal papers reporting on PET efforts of Year 3.



1. INTRODUCTION

1.1 The DoD High Performance Computing Modernization Program (HPCMP)

The Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) was instituted in 1994 to modernize the total high performance computational capability of the military research, development, test, and evaluation (RDT & E) community to a level comparable to that available in the foremost civilian and other government agency RDT & E communities. A key component of this initiative is the DoD Major Shared Resource Centers (MSRCs). This report summarizes the Program Environment and Training (PET) activities at the Army Corps of Engineers Waterways Experiment Station (CEWES) MSRC for year three of the contract which ran from 27 March 1998 though 26 March 1999.

The MSRCs provide complete HPC environments and include various types of computing systems, scientific visualization capabilities, extensive peripheral and archival storage, and expertise in use of these systems. The MSRCs support the wide variety of research and development problems arising from the science and technology programs supporting DoD's weapons development and war fighting support systems. The MSRCs provide the computer and computational sciences expertise to allow all the DoD laboratories to advance their capability in science and technology. The types of computer systems in the MSRCs are determined by user requirements and differ from one MSRC to another.

The HPCMP selected four DoD sites to become MSRCs:

- Army Corps of Engineers Waterways Experiment Station (CEWES), Vicksburg MS
- Army Research Laboratory (ARL), Aberdeen Proving Grounds MD
- Naval Oceanographic Office (NAVO), Stennis Space Center MS
- Air Force Aeronautical Systems Center (ASC), Wright–Patterson AFB, OH

In addition, DoD has identified ten Computational Technology Areas (CTAs) as being critical across DoD. The ten CTAs supported by the MSRCs are:

- CFD: Computational Fluid Dynamics
- CSM: Computational Structural Mechanics

- CCM: Computational Chemistry and Materials Science
- CEA: Computational Electromagnetics and Acoustics
- CWO: Climate/Weather/Ocean Modeling and Simulation
- SIP: Signal/Image Processing
- FMS: Forces Modeling and Simulation/C41
- EQM: Environmental Quality Modeling and Simulation
- CEN: Computational Electronics and Nanoelectronics
- *IMT*: *Integrated Modeling and Test Environments*

An integral part of the DoD HPCMP is the Programming Environment and Training (PET) at each MSRC by university/industry teams, which enables DoD researchers to develop and utilize the necessary HPC software. The PET program has training in the Computational Technology Areas (CTAs) and in relevant programming and technical infrastructure areas. Also, included is side-by-side transitioning of research codes into the MSRCs, as well as collaboration with MSRC users to advance and improve those codes.

The DoD HPCMP and the MSRCs are described more fully at the HPCMP website: http://www.hpcm.dren.net

2. CEWES MSRC PET STRATEGIC PLAN

The strategic plan of the CEWES MSRC PET effort has evolved over the first three years of operation, through close collaboration with the university team leadership, Nichols Research and the CEWES MSRC.

2.1 Goals and Objectives

The goal of the PET effort at the CEWES MSRC is to bring university HPC knowledge and skills to bear on the overall theme, Scalable HPC Applications and Performance, and specific sub-areas applicable to the CEWES MSRC.

The key goals of the PET effort in the CEWES MSRC are as follows:

- Establish a mechanism for identifying and transferring emerging advances in programming environments, computational tools, algorithms, and computational solution techniques for CTA applications from academia and industry into the CEWES MSRC.
- Create a virtual extension of the CEWES MSRC into academia that will be responsible for identifying and acquiring near-term programming environment improvements and long-term expansions, anticipating CEWES MSRC user needs, and making users aware of pertinent emerging technology.
- Utilize state-of-the-art HPC technology as an inherent part of the implementation of the CEWES MSRC PET Program itself.
- Establish a training program to ensure CEWES MSRC user proficiency with transferred advances in HPC tools and technology.
- Establish cooperative development and training programs with HBCUs/MIs to significantly enhance participation in the HPC community.
- Establish effective collaboration with academia to encourage the development of graduate and post-doc programs that will enhance the skill levels and efficiency of the DoD HPC community.

Based on this, the objectives for PET at CEWES MSRC are to:

• Transfer cutting edge, innovative HPC technology and tools from premier university centers to CEWES MSRC users and laboratories.

- Provide innovative collaborative environments for HPC research to all CEWES MSRC users ("remove importance of place").
- Train CEWES MSRC users in state-of-the-art HPC and scalable parallel processing (SPP) programming tools and techniques.
- Use HBCU/MI partners in an integral way to support PET objectives, enhance faculty and train minority students in HPC.
- Enable CEWES MSRC to make major productivity gains from current/planned hardware acquisitions.

The vision of the CEWES MSRC PET effort is a level of CEWES MSRC user capability and programming environment in the CEWES MSRC which is unsurpassed by academic, industry, or other government HPC centers.

2.2 Approach

The PET program at the CEWES MSRC combines a strong on-site team and a dedicated university team to constitute a virtual extension of the CEWES MSRC into top academic expertise. This team is able to respond and anticipate needs of the CEWES MSRC users for training and assistive collaboration in advancing the programming environment.

Support for CEWES MSRC users is provided by the PET team in the five Computational Technology Areas (CTAs) for which the CEWES MSRC has responsibility:

CFD: Computational Fluid Dynamics

CSM: Computational Structural Mechanics

CWO: Climate/Weather/Ocean Modeling and Simulation

EQM: Environmental Quality Modeling and Simulation

FMS: Forces Modeling and Simulation/C4I

and also for three relevant technical infrastructure areas:

Scalable Parallel Programming Tools

Scientific Visualization

Collaboration/Communication

The PET effort at CEWES MSRC consists of three fundamental elements: Core Support, Focused Efforts, and Training. Intertwined with these efforts are outreach to CEWES MSRC users and a program to enhance the involvement of HBCU/MIs in HPC.

Core Support provides continual interaction and assistive collaboration with CEWES MSRC users in the technical areas supported at the CEWES MSRC to migrate and enhance important codes to scalable parallel platforms and to extend the applicability of such codes and systems.

Focused Efforts address current specific projects to enhance the programming environment at the CEWES MSRC and the capabilities of CEWES MSRC users.

Training provides instruction for CEWES MSRC users, both on-site at CEWES MSRC and remote, in the technical areas supported at the CEWES MSRC and consists of both in-person and web-based courses.

2.3 Core Support

Core Support is provided to the CEWES MSRC through continual interaction in each of five CTAs supported at the CEWES MSRC, as well as in the three technical infrastructure support areas, with a specific supporting university on the PET team having responsibility for each area.

This Core Support operates primarily on-site at the CEWES MSRC coupled with continual support from specific individuals at the university; through continual interaction and assistive collaboration of the PET team with CEWES MSRC users to migrate important codes to scalable parallel platforms, and to enhance and extend the applicability of such codes and systems. In the operation of this Core Support, CEWES MSRC user demographics and software usage are continually monitored to provide input for identification of codes and systems of important impact.

2.4 Focused Efforts

Specific Focused Efforts within the scope of the CEWES MSRC and the resources of the PET effort are identified for implementation by the CEWES MSRC PET team, operating across the universities as necessary. Such projects have specific objectives and deliverables. When appropriate, projects involve coordinated

efforts among PET teams from other MSRCs and/or funding from other MSRC PET efforts. Interest by CEWES MSRC users in collaborating on such projects is a necessary factor in identification of Focused Efforts for implementation.

2.5 Training

Training is conducted with emphasis on intermediate and advanced topics, and is coordinated across the MSRCs to reach the entire DoD user community. A state-of-the-art training facility is maintained at the CEWES MSRC with workstations for hands-on training and facilities for remote transmission. Delivery is on-site at the CEWES MSRC, in person at other DoD sites, at the universities as appropriate, and remotely using emerging distance learning approaches. Training specifically addresses the need to reach a growing number of DoD users, leveraging emerging digital infrastructures and the unique educational expertise of the CEWES MSRC PET team. Delivery is ultimately to be any time, any place, and at any pace.

2.6 Outreach

Since the great majority of the CEWES MSRC users are off site, the PET effort at the CEWES MSRC places emphasis on outreach to remote users through visits to major remote user sites, training courses at remote sites, web-based remote training delivery, and remote communication via E-mail and the CEWES MSRC PET website. Emphasis is also placed on the implementation of appropriate tools for remote collaboration, especially with regard to scientific visualization. Continually updated user demographics are assembled into the CEWES MSRC user taxonomy to guide this outreach to the CEWES MSRC users.

2.7 HBCU/MI Program

The principal purpose of the HBCU/MI component of the PET effort at the CEWES MSRC is to enhance the capability of the HBCU/MI members of the CEWES MSRC PET academic team to participate fully in the PET support effort of the CEWES MSRC. To this end, both Jackson State University and Clark Atlanta University are involved directly in Focused Efforts. Particular emphasis is placed on enhancing the opportunities of students at the HBCU/MI PET partners through web-based university classes at the HBCU/MIs from the other PET team members and through summer institutes at the HBCU/MIs.

3. IMPLEMENTATION

3.1 Management

The CEWES MSRC PET effort is administered by the integrator, Nichols Research Corporation (NRC), for the CEWES MSRC as a part of the CEWES MSRC contract. Dr. Dick Pritchard of Nichols Research was the PET Director through June 12, 1998. Ray Burgess of NRC is the Acting PET Director. Prof. Joe Thompson of Mississippi State University is CEWES MSRC PET academic team leader. Dr. Wayne Mastin of Nichols, and a professor emeritus of Mississippi State University, is the on-site PET team leader. Prof. Willie Brown of Jackson State University is the HBCU/MI leader. Dr. Louis Turcotte of the CEWES MSRC exercises oversight of the CEWES MSRC PET effort for the government.

3.2 Organization

The fundamental mode of operation for PET at the CEWES MSRC is a direct and continual connection between the CEWES MSRC users and the CEWES MSRC PET team universities in support of the five Computational Technology Areas (CTAs) supported at the CEWES MSRC and three related technical infrastructure areas. This is accomplished through a combination of full-time university and NRC personnel on-site at the CEWES MSRC, in close communication with faculty members at the university with partial-time commitment to the CEWES MSRC PET effort for support and leadership.

3.3 Team Composition

The university PET team for the CEWES MSRC is led by the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University, with Jackson State University as the lead HBCU/MI. The university team is as follows:

Center for Computational Field Simulation – ERC (NSF Engineering Research Center at Mississippi State University)

Jackson State University

National Center for Supercomputing Applications – NCSA (NSF PACI Center at the University of Illinois)

Center for Research in Parallel Computing – CRPC (NSF Science and Technology Center headquartered at RiceUniversity)

Northeast Parallel Architectures Center – NPAC (at Syracuse University)

Ohio State University and Ohio Supercomputer Center – OSC (at Ohio State University)

Innovative Computing Laboratory – ICL (at University of Tennessee Knoxville)

Texas Institute for Computational and Applied Mathematics – TICAM (at University of Texas at Austin)

University of Southern California

Clark Atlanta University

Dedicated on-site/at-university support teams for each of the five DoD Computational Technology Areas (CTAs) supported at the CEWES MSRC were the responsibility of specific universities on the PET team at the CEWES MSRC in Year 3:

- CFD: Computational Fluid Dynamics ERC (Mississippi State)
- CSM: Computational Structural Mechanics –ERC (Mississippi State)
- CWO: Climate/Weather/Ocean Modeling and Simulation OSU (Ohio State)
- EQM: Environmental Quality Modeling and Simulation TICAM (Texas)
- FMS: Forces Modeling and Simulation/C4I NPAC (Syracuse)

as were each of the following three technical infrastructure support areas:

- Scalable Parallel Programming Tools CRPC (Rice) and ICL (Tennessee)
- Scientific Visualization NCSA (Illinois)
- *Collaboration/Communication NPAC (Syracuse)*

Mississippi State, Ohio State, Texas, and Rice maintain on-site university personnel at the CEWES MSRC in support of CFD (Dr. Steve Bova – MSU), CSM (Dr. Rick Weed – MSU), CWO (Dr. Steve Wornom – Ohio State), EQM (Dr. Phu Luong – Texas) and Scalable Parallel Programming Tools (Dr. Clay Breshears – Rice). NRC has a person on-site in support of Scientific Visualization (Dr. Richard Strelitz – SAIC). NRC also has a Training Coordinator (John Eberle – NRC) on-site.

3.4 Reporting and Technology Transfer

Transfer of emerging technology from the academic community into the CEWES MSRC is a primary purpose of the CEWES MSRC PET effort. Of like importance is transfer in the other direction, providing input and feedback regarding emerging DoD needs to influence developments at universities. The primary mode of technology transfer in the CEWES MSRC PET effort is direct contact between the PET team and the CEWES MSRC users. However, the PET team produces a series of reports on technology developments for distribution to CEWES MSRC users. Also, technology transfer is a prime emphasis of the training component of the CEWES MSRC PET effort. The on site personnel at the CEWES MSRC from the PET team form a continual conduit for technology transfer.

This page intentionally left blank

4. TECHNICAL SUPPORT TEAMS

The fundamental mode of operation for the PET support effort at the CEWES MSRC is a direct and continual connection between the CEWES MSRC PET team universities and the CEWES MSRC users in support of the five Computational Technology Areas (CTAs) supported at the CEWES MSRC and three related technical infrastructure areas.

This is accomplished through on-site PET team members at the CEWES MSRC in close communication with PET team members at the supporting universities, who also make frequent visits to CEWES MSRC. The PET team members on-site at CEWES MSRC are full-time university personnel, supplemented by NRC personnel. The on-site PET team members at the CEWES MSRC are key to the CEWES MSRC PET operation, since these team members are the front line of contact with CEWES MSRC users.

These seven on-site team members are as follows:

Lead: Dr. Wayne Mastin - NRC (Professor Emeritus of Mississippi State)

CFD: Dr. Steve Bova - Mississippi State

CSM: Dr. Rick Weed - Mississippi State

CWO: Dr. Steve Wornom - Ohio State

EQM: Dr. Phu Luong - Texas

SPP Tools: Dr. Clay Breshears - Rice

SV: Dr. Richard Strelitz - NRC (SAIC)

Also on-site at CEWES MSRC are the overall PET Project Leader – Dr. Dick Pritchard for part of Year 3 and Ray Burgess as interim - and the Training Coordinator, John Eberle, all of NRC. During part of Year 3, Dr. Bob Fithen of Texas was on-site in support of EQM, but left for an academic career, being then replaced by Dr. Phu Luong of Texas. A complete listing of all the CEWES MSRC PET team personnel is given in Table 1.

During Year 3, the eight technical support teams in the CEWES MSRC PET effort operated as shown in the following paragraphs.

4.1 CFD: Computational Fluid Dynamics CTA (ERC – Mississippi State)

CFD support in the PET effort at CEWES MSRC is the responsibility of the NSF Engineering Research Center for Computational Field Simulation at Mississippi State University. During the third contract year, the CFD support team consisted of Prof. David Huddleston (Senior Academic Lead), Dr. Steve Bova (On-site Lead), Prof. Jianping Zhu and Mr. Purushotham Bangalore. The On-site Lead (Bova) serves as an effective administrative liaison between CEWES MSRC, NRC, and MSU, and as a technical liaison between CEWES MSRC users and the entire CFD support team. Bova also coordinates communication and facilitates interaction with other components of the CEWES MSRC PET team. This includes maintenance of the CFD Web page content and biweekly activity reporting.

The CFD team in the CEWES MSRC PET effort serves the CEWES MSRC by providing:

Program-wide CFD support.

R & D expertise on selected technology enhancements.

HPC assistance for targeted codes.

Program-wide support pertains to direct CEWES MSRC user contact and cultivation, participation in workshops and technical meetings, user training in HPC, and other generic duties. HPC support for targeted codes and delivery of collaborative R & D expertise are more specific tasks selected to provide technology that has potential application and interest throughout the CEWES MSRC user community. Year 3 support was structured such that the On-Site Lead assumed primary responsibility for user contact and interaction. Primary contributions of the at-university team were through focused effort collaboration among the MSU CFD team, the CWO team at OSU, and CEWES MSRC users with responsibility of developing a parallel implementation of the CH3D-SED solver.

4.2 CSM: Computational Structural Mechanics CTA (TICAM - Texas, with ERC - Mississippi State)

CSM support in the PET effort at CEWES MSRC is the responsibility of TICAM (Texas Institute for Computational and Applied Mathematics) at the University of

Texas at Austin. The CSM team is led by Prof. J. Tinsley Oden and Prof. Graham F. Carey as Senior Academic Leaders. Dr. David Littlefield (IAT-Texas) is a major research contributor and works closely with the CTH Application group (G. Hertel, D. Crawford) at Sandia. Dr. Abani Patra (University of Buffalo) and Dr. Atanas Pehlivanov (Texas) have been conducting studies related to EPIC. Dr. Robert McLay (Texas) is working with Littlefield on the design of a software testbed to evaluate indicators and algorithms for incorporation in CTH. Oden and Carey are carrying out research (with the team members) on error indicators and adaptive strategies to support the effort. On-site support at CEWES MSRC, including concentration on user contacts, is provided by the CSM On-Site Lead, Dr. Rick Weed of the ERC at Mississippi State, working in close contact with the Texas group.

4.3 CWO: Climate/Weather/Ocean Modeling and Simulation CTA (Ohio State)

The CWO CEWES MSRC support team consists of the PET On-Site Lead (Dr. Steve Wornom), two Senior Academic Leaders (Prof. P. Sadayappan and Prof. Keith Bedford), a research scientist (Dr. David Welsh) and a graduate research associate. We have an informal advisory group of CEWES MSRC scientists lead by Bob Jensen, with additional contributions from Joe Gailani and Billy Johnson, and less frequent contacts with J. McKee-Smith and Jeff Holland. The functions of this group are to review the contributions the OSU team makes, develop goals and strategies for future work, and advise on content for workshops and training classes. The union of the OSU CWO team and MSRC users is considered to be the complete CWO team.

The OSU team is responsible for implementing the goals of the annual CEWES MSRC PET CWO projects, and the team internally pursued these goals in the following way during Year 3. Project supervision, reporting, and proposal preparation were the province of Sadayappan and Bedford. The training portion of our work was the primary responsibility of Welsh and another research scientist (Dr. Shuxia Zhang held this position until 9/98), with on-site instruction assistance from Bedford and Sadayappan. The core support code enhancements to WAM, SWAN and FBM were the responsibility of Welsh and Wornom, while the focused effort on coupling was implemented by Zhang and Welsh, the graduate student, and Sadayappan and Bedford. The focused effort on CH3D-SED, in collaboration with the CFD team from MSU, was handled by Zhang and the graduate student. Daily to weekly staff meetings (including conference calls with Wornom) were the primary means of internal coordination and communication.

CWO interactions were handled in the following way. For the major portion of Year 3, Welsh served as the virtual PET on-site staff and made frequent trips to CEWES MSRC to coordinate with CEWES MSRC staff. These meetings also included Sadayappan and Bedford when leveraging of their trips to CEWES MSRC was possible. At the end of January 1999, this virtual staff approach was terminated when Wornom became the CWO On-Site Lead. With regard to other forms of communication, all the OSU staff assisted with E-mail and telephone contact with CEWES MSRC personnel and the other on-site staff, and in the preparation of the biweekly Web reports, annual reports, and PET Technical Reports.

4.4 EQM: Environmental Quality Modeling and Simulation CTA (TICAM - Texas)

EQM support in the PET effort at CEWES MSRC is the responsibility of TICAM (Texas Institute for Computational and Applied Mathematics) at the University of Texas at Austin. The CEWES MSRC PET EQM team for Year 3 consisted of Prof. Mary F. Wheeler, Prof. Clint Dawson, Dr. Victor Parr, Dr. Jichun Li, Dr. Robert Fithen, Robert Kirby, Dr. Monica Martinez and Steve Cutchin. Wheeler is the Senior Academic Leader. Dawson, Li, Martinez, Kirby and Cutchin worked on various aspects of the project at the University of Texas at Austin. Fithen was the EQM On-Site Lead from June of 1998 until he left in August of 1998 to take a faculty position. He has been replaced by Dr. Phu Luong. Parr served as EQM user liaison and was in frequent contact with both the Texas personnel and with EQM personnel at CEWES.

4.5 FMS: Forces Modeling and Simulation/C4I CTA (NPAC - Syracuse)

The CEWES MSRC PET FMS support team is based at the Northeast Parallel Architectures Center (NPAC) at Syracuse University. Within NPAC, FMS activities are centered around the Interactive Web Technologies (IWT) Group led by Dr. Wojtek Furmanski. The group includes two research scientists and roughly a dozen graduate research assistants who make various contributions to the FMS activities.

4.6 C/C: Collaboration and Communications (NPAC - Syracuse)

The Northeast Parallel Architectures Center (NPAC) at Syracuse University provides most of the team that supports the Collaboration and Communications (C/C) technical infrastructure area. The Syracuse team is led by NPAC's Director, Prof. Geoffrey C. Fox, and draws as necessary on the wide range of C/C-related

capabilities represented by NPAC's research staff and students. Principal contributions to the support effort during Year 3 came from Dr. David Bernholdt, the TANGO Interactive Collaboratory Group headed by Dr. Marek Podgorny, and Yuping Zhu, drawing on her background in Web-linked databases and intranets. Day-to-day C/C operations, such as the PET Web site and the TANGO Interactive server, were handled by NRC on-site staff members Herman Moore and John Eberle, respectively.

4.7 SPP Tools: Scalable Parallel Programming Tools (CRPC – Rice and ICL - Tennessee)

The CEWES MSRC PET Scalable Parallel Programming Tools (SPP Tools) support team is based at the Center for Research on Parallel Computation (CRPC), an NSF-funded Science and Technology Center with headquarters at Rice University. Rice plays the lead role in SPP Tools at CEWES MSRC as well. The Innovative Computing Laboratory (ICL) at the University of Tennessee at Knoxville also has a major role in SPP Tools at CEWES MSRC. The goal of the CRPC is "to make parallel computing truly usable by scientists and engineers". Toward this end, CRPC researchers have assessed the software and algorithmic problems posed by parallel and distributed machines. The solutions they have found are crucial elements of the PET support effort in the DOD HPC Modernization Program. In addition, team members have led a number of significant standards efforts, including the High Performance Fortran (HPF) Forum, Message Passing Interface (MPI) Forum, the BLAS Technical Forum, and ParkBench.

Key personnel involved in the CEWES MSRC PET SPP Tools effort are Prof. Ken Kennedy (Senior Technical Lead, Rice University), Prof. Jack Dongarra (Senior Technical Lead, Tennessee), Dr. Dick Hanson (SPP Tools Lead, Rice University, starting 1-1-99), Dr. Shirley Browne (SPP Tools Lead, Tennessee), Dr. Clay Breshears (On-site SPP Tools Lead, Rice), and Dr. Ehtesham Hayder (Rice). Dr. Chuck Koelbel (Rice) was the SPP Tools Lead until leaving in August for NSF.

The SPP Tools Team members use informal electronic means (E-mail and telephone) to communicate at a distance. Typically other contacts are driven by specific projects or focused efforts. For example, a CEWES MSRC user will request a new tool through his on-site CTA lead, by contacting Breshears. Breshears will relay the request to one of the universities for advice, contacting the team member with the most experience in the specific area. Usually, a pointer to useful software will be forthcoming in short order. The team does not follow a strict command structure, but finds that cooperating in this way is very effective.

They also meet a few times a year at conferences such as the DOD HPCMP Users Group Meeting to exchange ideas and related experiences.

The Tennessee SPP Tools team is drawn from researchers and graduate students who make up the Innovative Computing Laboratory (ICL), a research group of over forty people under the direction of Distinguished Professor Jack Dongarra. ICL has internationally recognized expertise in the areas of parallel linear algebra and high performance math software, parallel and distributed inter-process communication, and performance evaluation and optimization. ICL has produced the widely used high-quality LAPACK and ScaLAPACK linear algebra libraries, as well as the PVM and NetSolve parallel computing systems. Several of the ICL research staff spend a significant portion of their time working on CEWES MSRC PET projects and core support activities. In addition, any of the ICL staff are available for short-term consulting as needed.

4.8 SV: Scientific Visualization (NCSA - Illinois, with ERC - Mississippi State)

The PET Scientific Visualization (SV) team for the CEWES MSRC is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois, with additional support from the ERC at Mississippi State. Dr. Polly Baker (NCSA) serves as Senior Academic Lead, providing long-term direction and leadership for the effort. Dr. Alan Shih (NCSA) serves as NCSA project lead. Dr.Shih is headquartered at NCSA but spent a significant amount of his time at the CEWES MSRC during Year 3. Prof. Robert Moorhead (MSU) and Prof. Raghu Machiraju (MSU) also served as project leads during Year 3. Dr. Richard Strelitz (NRC-SAIC) serves as primary liaison between the CEWES MSRC and the academic personnel.

The team also included project developers at NCSA, including Randy Heiland, Dave Bock, and Rob Stein. Project developers from MSU included Mike Chupa, Kelly McCarter, and Cass Everitt (working with Prof. Moorhead) and Bala Nakshatrala (working with Prof. Machiraju).

The PET SV team interacts with CEWES MSRC users to define user needs, provide information on available solutions, and prototype custom solutions where necessary. The team also coordinates with other CEWES MSRC personnel specializing in visualization.

5. YEAR 3 MAJOR ACCOMPLISHMENTS

As has been noted above, the PET effort at the CEWES MSRC operates through providing core support to CEWES MSRC users, performing specific focused efforts designed to introduce new tools and computational technology into the CEWES MSRC, conducting training courses and workshops for CEWES MSRC users, and operating an HBCU/MI enhancement program.

The major accomplishments of the CEWES MSRC PET effort in enhancing the programming environment at the CEWES MSRC during Year 3 are described in this section. The presentation here is according to CTAs and technical infrastructure support areas, but there is much overlap in effort.

Tools introduced into the CEWES MSRC in the course of Year 3 of the PET effort are listed in Table 4, and are described in Section 6. Specific CEWES MSRC codes impacted by the PET effort during Year 3 are listed in Table 5, and items of technology transfer into the CEWES MSRC are listed in Table 6. More detail on the Year 3 effort is in the CEWES MSRC PET Technical Reports and other publications from Year 3 that are abstracted in Section 10. Training conducted during Year 3 is described in Section 7, and general support of CEWES MSRC users is covered in Section 8. The accomplishments in the HBCU/MI component of the CEWES MSRC PET effort are discussed in Section 9.

5.1 CFD: Computational Fluid Dynamics CTA (ERC - Mississippi State)

Primary core support contributions were made during Year 3 by the On-Site Lead (Bova) with overall coordination assistance from the at-university team. One Focused Effort, Scalable and Parallel Integration of Hydraulic, Wave, and Sediment Transport Models, was conducted during Year 3.

5.1.1 Parallel CGWAVE

A dual-level parallel algorithm using both MPI and OpenMP was designed and implemented into the CGWAVE solver supporting Zeki Demirbilek of CEWES. This resulted in dramatic reduction in turnaround time. Turnaround time for the demonstration case was reduced from 2.1 days to 12 minutes using 256 SGI O2000 processors. This project, which also served



Figure 5-1. CEWES MSRC HPC Challenge Team at SC98 in Orlando

as a test bed for the MPI_Connect Tool implemented by the Tennessee SPP Tools team in PET, was initiated through user interaction at one of the Bring Your Own Code (BYOC) workshops and was selected as the "Most Effective Engineering Methodology" in the HPC Challenge at SC98.

5.1.2 Parallel CH3D/SED

In Year 3, the Focused Effort, Scalable and Parallel Integration of Hydraulic, Wave and Sediment Transport, was initiated in collaboration with the PET CWO team at Ohio State. The purpose of this focused effort was to enhance national defense and security by

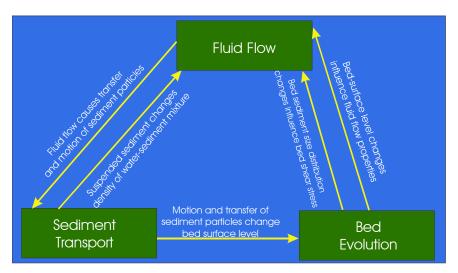


Figure 5-2. Model of fluid flow with sediment transport

developing a scalable, parallel implementation of a coupled wave (WAM), hydraulic (CH3D) and sediment transport (SED/COSED) simulation code. Once developed, this code will enable more accurate and efficient evaluation of DoD applications such as naval harbor access, wind/wave hazard forecasting, coastal forecasts for amphibious operations, in addition to various civil works applications. Stronger coupling of these technologies through this project will result in a simulation capability including more realistic representation of the interaction between surface and bottom shear stresses that will improve representation of physical phenomena. Parallelization and HPC support will substantially reduce computational requirements for long period simulations and allow more timely simulation of configurations of military interest.

Task responsibilities within this focused effort were distributed between the CFD and CWO teams. In Year 3, the primary contribution of the CFD team was development of a parallel implementation of the CH3D solver, including the non-cohesive sediment model (SED), and computer science support on model integration.

CEWES MSRC user constraints require results from the parallel solver to replicate results from the unmodified sequential solver within machine accuracy, and that input and output files be compatible with sequential versions. Consequently, the implemented parallelization strategy utilized a three-stage approach: pre-processing and partitioning, parallel computation, and post-processing. During the pre-processing and partitioning phase, the grid is partitioned using a simple load-balancing technique to obtain roughly equal number of computational cells per processor, with separate grid files generated for each processor along with the other necessary input files. All the processors perform the computation in parallel and exchange data at the processor boundaries in the parallel computation phase. At the end of a simulation, each processor writes the corresponding part of the solution to disk. These individual files are later merged during the post-processing stage to generate output files suitable for visualization.

To verify the accuracy of the parallelization effort, simulations were performed on two different test cases. Verification of parallel CH3D/SED was done in close collaboration with the CWO team and CEWES personnel. Test case 1 was tested on the SGI Origin 2000 and the CRAY T3E for different numbers of processors, and the performance was analyzed. Significant reduction in the execution times was observed up to 32 processors. Test case 2 was tested for various numbers of processors, and a more long-term (in the time dimension) simulation was performed. Details of the code scalability performance and verification are included in the final report on this effort.

The impact of this work on CEWES MSRC is to significantly reduce the time required for high-resolution sediment transport simulations by making use of the scalable nature of the high performance computing facilities. This work was also essential for the development of a scalable coupled model of hydraulic, sediment, and wind-wave processes, which greatly affects military operations in the marine environment.

5.2 CSM: Computational Structural Mechanics CTA (TICAM - Texas, with ERC - Mississippi State)

The CSM core support and focused efforts constitute a cohesive approach that includes the Texas CSM team, the Army Institute for Advanced Technology (at Texas) activities, Sandia applications and software development, and CEWES MSRC applications using CTH and EPIC. The work has a strong impact on DoD applications and CEWES MSRC since it promises to change the entire approach for solving these problems in a timely and more reliable way.

The principal goal of the TICAM CSM support in the CEWES MSRC PET effort is to introduce, implement and test adaptive grid techniques for analysis of CSM problems for DoD simulation of "violent events". Representative DoD codes include CTH and EPIC. This work requires consideration of the following:

Appropriate a posteriori error estimates and corresponding indicators for these problem classes.

Strategies for h, (p and hp) adaption of the grid.

Complications in implementing the adaptive schemes related to the form of "legacy code".

Development and incorporation of appropriate data structures for adaptive refinement and coarsening.

Efficiency in implementation.

Parallel, scalable HPC needs.

CSM core support and focused effort activities on the project have been targeted to these goals, and we have made several significant progress accomplishments, as represented in the two efforts related to CTH and EPIC described below. This work has been closely coordinated with our core support activities. In addition, we have worked closely with Sandia researchers and made three working trips to Sandia to foster the collaboration and expedite the work. Carey has been interacting with Rob Leland's group at Sandia on grid partitioning, grid quality, and parallel partitioning issues. Following his February visit to Sandia the group obtained the CHACO software and has implemented it at Texas. We are currently experimenting with this partitioning software and will be incorporating our space-filling curve scheme into it.

Both of these studies are singular accomplishments since they are, we believe, the first adaptive refinement calculations for this class of applications codes. They therefore constitute a strong statement concerning the main program goal — to introduce and tech transfer advanced adaptive grid strategies from the university and research labs to the DoD application groups.

5.2.1 CTH: Block Adaptive Strategy

We have developed a block adaptive strategy in collaboration with Sandia and have carried out some preliminary simulation studies. This work has been implemented as an extension of the CTH code.

Here the test problem corresponds to hypervelocity impact of a spherical copper projectile with a target. The number of cells in the adaptive simulation are approximately one-third that of a comparable uniform grid simulation that yields the desired fine mesh resolution. As part of the work, we are also developing new error and feature indicators to guide refinement and assess computational reliability.

5.2.2 EPIC: Simplex Refinement Strategy

We have developed a local simplex refinement strategy and implemented it in the test code EPIC (Elasto-Plastic Impact Computation). As the simulation proceeds, elements are locally refined based on element feature and error indicators. Preliminary numerical tests have been carried out for the "Taylor Anvil" problem to assess the utility of the approach. Related work on space-filling curves for mesh partitioning and on grid quality is also being carried out.

5.3 CWO: Climate/Weather/Ocean Modeling and Simulation CTA (Ohio State)

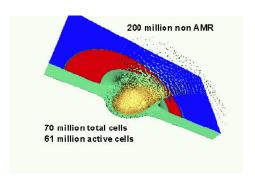


Figure 5-3. Adaptive CTH simulation of copper ball impacting a steel plate

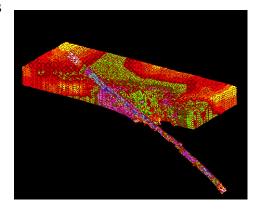


Figure 5-4. EPIC simulation of a rod penetrating a plate

The rationale for the CWO team in the CEWES MSRC PET effort, and the evolution of its effort over the last three years continues to be based on the following three points:

First, and most importantly, DoD has an extremely urgent need for timely (forecasted) information about hazardous and mitigating conditions in its theaters of interest. The primary classes of problems encountered include the following: the prediction of extreme wave conditions for fleet operations both offshore and in nearshore regions; the maintenance of port and harbor navigability and associated inlet conditions; the prediction of ocean sediment storms in the North Atlantic for finding enemy submarines or providing camouflage for our submarines; improved prediction of acoustic waveguides; and integrated systems for predicting subsurface mine burial mechanics and weapons retrieval. One land-based

extension of these activities is the prediction of sandstorms for desert troop operations.

Second, these problem areas have several common threads. The hazardous conditions are extreme in magnitude and infrequent in occurrence, are forced by associated atmospheric events, result from three-dimensional turbulent fluid dynamics with a very broadband spectrum of nonlinearly interacting processes, give rise to sediment resuspension and transport, and most often occur in regions of shallow water or irregular coastline geometry.

Third, the present modeling strategies which underlie the forecasting procedures for these problems consist of isolated models of the various processes which are not well linked and, therefore, not able to resolve the most extreme and, consequently, the most important information that DoD needs from the forecasting programs.

5.3.1 Integrated Coastal Modeling Systems (ICOMS)

The basis of the CWO program in PET at CEWES MSRC is to implement the new model structures and couplings necessary to allow the prediction of these extreme rapid but infrequent events, especially in the nearshore, embayment, and continental shelf environments. The increased scope and size of these new Integrated Coastal Modeling Systems (ICOMS) cannot be achieved without the use of highly parallelized software executed on highly parallel machines.

During the first two years, we have been able to proceed on two fronts: the first being the parallelization and improvement of the individual codes that are to be integrated into ICOMS, and the second being the creation of the model physics, structural, and software improvements, as well as the message passing structures, necessary to begin full coupling of wave, circulation and sediment transport codes for these integrated predictions.

The individual code improvements in Year 3 centered on the completion of the parallelization and performance benchmarking of the WAM code for shallow water wave prediction, and the SED code (in collaboration with the CFD team at MSU) for noncohesive sediment resuspension and transport calculations. These activities are complete. Coupling improvements completed in Year 3 included implementation of the unsteady current refraction and radiation stress physics necessary to couple the WAM wave and CH3D circulation models. The SED model was also fully coupled except for the bottom boundary conditions.

In Year 3, we have completed the coupling of the wave, circulation and noncohesive sediment transport codes and performed preliminary verification. The coupling yielded results that are significantly improved in the nearshore zone, and the tests for an extremely challenging storm, wave, and sediment plume event were quite satisfactory. Tasks remaining for Year 4 include full atmospheric model coupling, the completion of the sediment bottom boundary layer conditions, and the application of ICOMS to an area of DoD interest.

5.4 EQM: Environmental Quality Modeling and Simulation CTA (TICAM - Texas)

In Year 3, the EQM team's core and focused efforts involved continuing parallel EQM code migration, developing new algorithms and software for coupling hydrodynamic flow and transport simulators, developing new software for launching parallel codes from the Web, and providing user training through frequent personal contact, workshops, and conferences.

5.4.1 Parallel CE-QUAL-ICM

The EQM team continued its efforts in the parallel migration of CE-QUAL-ICM. In Year 2, parallel version 1.0 of CE-QUAL-ICM was developed. In Year 3, a number of improvements were added to the code, resulting in version 2.0. In particular, the code is now able to run on any number of processors (before it was limited to 32 processors due to the way I/O was being handled) and the overall file I/O was improved. The mesh partitioning strategy was also improved through the use of PARMETIS, a parallel mesh partitioning code developed at the Army High Performance Computing Research Center (AHPCRC) at Minnesota. Overall, version 2.0 is roughly 25% faster than version 1.0. During Year 3, CEWES MSRC users Carl Cerco, Mark Noel and Barry Bunch have run 106 10-year simulations. In the same amount of wall clock time, they would have been able to run only 11 scenarios with the previous serial version. Thus, the parallel code has resulted in an increase of an order-of-magnitude in computing capability and is now being used for production simulation.

5.4.2 Parallel ADCIRC

During Year 3, the EQM team migrated the finite element hydrodynamics code ADCIRC (Advanced Circulation Model) to the CEWES MSRC parallel platforms. The same general parallelization approach that was used to parallelize CE-QUAL-ICM was employed. In particular, a preprocessing code was created which splits the global finite element mesh and global data into local datasets for each processor. Here mesh partitioning algorithms based on space-filling curves and the PARMETIS code were investigated. The latter code greatly improved the

parallel performance for large numbers of processors. The parallel code was

tested on several large datasets. For one dataset with 271.240 nodes a speedup of 169 on 256 processors of the CRAY T3E was obtained. Speedups on smaller numbers of processors was almost linear with the number of processors. Improved versions of ADCIRC including wetting/drying and three-dimensional effects are under development, and the EOM team continues to consult with CEWES MSRC users on the parallelization of the code.

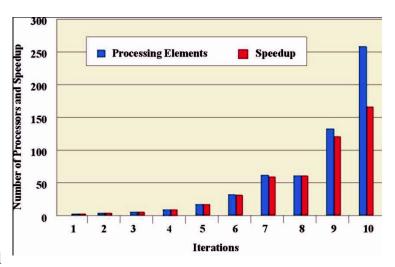


Figure 5-5. Number of processors and speedup for parallel ADCIRC computations on CRAY T3E

5.4.3 Coupling ADCIRC and CE-QUAL-ICM: Projection –UTPROJ

One of the EQM team's major efforts in Year 3 was in the development of a projection algorithm and software for coupling hydrodynamics and water quality models. In this coupling, the major issue is in providing a mass conservative velocity field suitable for the finite volume method used in CE-OUAL-ICM. We developed and implemented such an algorithm in the code UTPROJ. Theoretical error estimates for the methodology were derived which show that the projected velocities, besides being mass conservative, are at least as accurate as the original velocities produced by the hydrodynamics code. A two-dimensional code was first developed to show proof of concept. Simultaneously, a similar two-dimensional code, PROFEM, was developed at CEWES. Comparisons between UTPROJ and PROFEM led to changes in the PROFEM solver, speeding it up by an order-of-magnitude. We extended UTPROJ to three dimensions during Year 3 and have tested it on some synthetic datasets. The three-dimensional code is very general, allowing for combinations of tetrahedral, prismatic and hexahedral elements. To make it a truly usable code, further testing, parallelization, and improvements to the linear solver are planned for Year 4.

A prototypical demonstration of the coupling capability between ADCIRC and CE-QUAL-ICM using UTPROJ was performed during Year 3. Circulation in

Galveston Bay was first simulated using the parallel ADCIRC code. The output from this code (elevation, velocities) for each transport time step was projected onto the same grid. Movement of a contaminant was then performed using a transport code similar to CE-QUAL-ICM that we developed. A scenario whereby a point source of contaminant is released into the bay was simulated. At present, the links between flow, projection and transport are primitive. During Year 4, we hope to vastly improve the coupling process, so that it is seamless to an EQM CEWES MSRC user.

5.4.4 Transport Schemes on Unstructured Meshes: CE-QUAL-ICM

In conjunction with our activities related to water quality modeling, the EQM team investigated and implemented second-order accurate transport schemes suitable for unstructured grids. This is motivated by the need to extend the second-order QUICKEST scheme currently used in CE-QUAL-ICM to unstructured, three-dimensional grids for planned future CEWES applications. A two-dimensional code has been developed on triangular grids, and a number of different algorithms are being tested in this framework.

5.4.5 Web Launching: PARSSIM

The EQM team also had a focused effort on Web launching in Year 3. The launching capability was demonstrated using the PARSSIM subsurface transport simulator, a parallel code developed at Texas. A client Java applet with GUI (graphical user interface) and three-dimensional visualization capabilities was created that allows remote users to access the PARSSIM code and data domains on CEWES MSRC servers. The results of the computation are saved on the

CEWES MSRC local disks and can be selectively retrieved from Java visualization applets. The Java applet can be initiated from any Internet Web browser. As a first prototype of launching, we created tools appropriate for launching PARSSIM and/or a visualization server selectively on CEWES MSRC server machines. An outstanding task is to incorporate GLOBUS support to support metacomputing on multiple workstations.

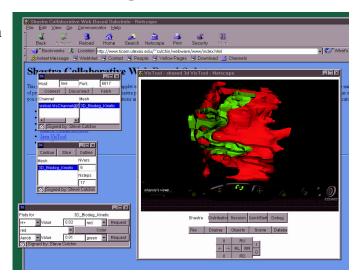


Figure 5-6. GUI for launching the simulation code PARSSIM

5.5 FMS: Forces Modeling and Simulation/C4I CTA (NPAC - Syracuse)

Year 3 FMS effort in PET at CEWES MSRC can be divided into two distinct but related thrusts. The major effort continued the core development of our WebHLA framework, and we also developed and delivered demonstrations of its use with specific FMS applications, such as parallel CMS (Comprehensive Mine Simulator). Another effort used some of the tools and technologies that underlie WebHLA (i.e. WebFlow, CORBA) to provide an environment, which facilitates the integration of multiple simulation applications under Web-based user interfaces.

5.5.1 WebHLA Activities

WebHLA follows the 3-tier architecture of our Pragmatic Object Web, with a mesh of JWORB(Java Web Object Request Broker)-based middleware servers managing back-end simulation modules and offering Web portal style interactive multi-user front-ends. JWORB is a multi-protocol server capable of managing objects conforming to various distributed object models including CORBA, Java, COM and XML. HLA is supported via Object Web RTI (OWRTI), i.e. Java/CORBA-based implementation of DMSO RTI 1.3, packaged as a JWORB service. Distributed objects in any of the popular commodity models can be naturally grouped within the WebHLA framework as HLA federates, and they can

naturally communicate by exchanging (via JWORB-based RTI) XML-ized events or messages packaged as some suitable FOM interactions.

HLA-compliant M&S systems can be now integrated in WebHLA by porting legacy codes (typically written in C/C++) to suitable HPC platforms, wrapping such codes as WebHLA federates using cross-language (Java/C++) RTICup API, and

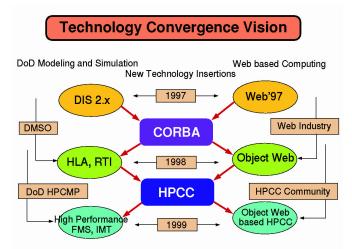


Figure 5-7. Integration of commodity web technology for distributed objects with DMSO/RTI

using them as plug-and-play components on the JWORB/OWRTI software bus. In case of previous generation simulations following the DIS (or ALSP) model, suitable bridges to the HLA/RTI communication domain are now also available in WebHLA, packaged as utility federates. To facilitate experiments with

CPU-intense HPC simulation modules, we developed suitable database tools such as event logger, event database manager and event playback federate that allow us to save the entire simulation segments and replay later for some analysis, demo or review purposes. Finally, we also constructed SimVis — a commodity (DirectX on NT) graphics-based battlefield visualizer federate that offers a real-time, interactive, 3D front-end for typical DIS HLA entity level (e.g. ModSAF style) simulations.

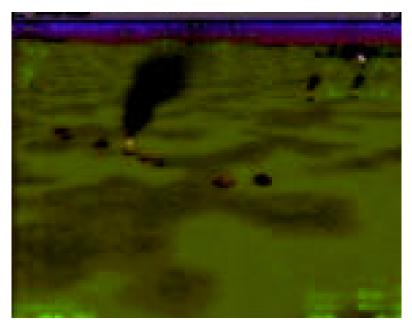
In parallel with prototyping core WebHLA technologies such as JWORB or OWRTI, we are also analyzing some selected advanced M&S modules such as the CMS (Comprehensive Mine Simulator) system developed at Ft. Belvoir VA that simulates mines, mine fields, minefield components, standalone detection systems and countermine systems including ASTAMIDS, SMB and MMCM. The system can be viewed as a virtual T&E tool to facilitate R&D in the area of new countermine systems and detection technologies of relevance both for the Army and the Navy. We recently constructed a parallel port of the system to the Origin2000, where it was packaged and can be used as either a DIS node or as an HLA federate.

Based on the analysis of the sequential CMS code, we found the semi-automatic, compiler directives based approach as the most practical parallelization technique to start with in our case. The most CPU-intensive inner loop of the CMS simulation runs over all mines in the system, and it is activated in response to each new entity state PDU to check if there is a match between the current vehicle and mine coordinates that could lead to a mine detonation. Using directives such as "pragma parallel" and "pragma pfor" we managed to partition the mine-vehicle tracking workload over the available processors, and we achieved a linear speedup on up to four processors. For large multi-processor configurations, the efficiency of our pragma-based parallelization scheme deteriorates due to the NUMA memory model and increased contention on the internal network. This makes efficient use of cache critically important to obtaining scalable performance. We were unable to enforce a cache-efficient data decomposition using pragmas, probably due to the rather complex object oriented and irregular code in the CMS inner loop. We are currently rebuilding and simplifying the inner loop code so that the associated memory layout of objects is more regular and hence predictable.

Playing the real scenario over and over again for testing and analysis is a time consuming and tedious effort. A database of the equivalent PDU stream would be a good solution for selectively playing back segments of a once-recorded scenario. For a prototype version of such a PDU database (PDUDB) we used Microsoft's Access database and Java servlets for loading as well as retrieving the data from the database using JDBC. The PDU logger servlet receives its input via an HTTP

PORT message in the form of XML-encoded PDU sequences. The input stream is decoded, converted to SQL and stored in the database using JDBC. The playback is done using another servlet that sends the PDUs generated from the database as a

result of a query. The servlet is activated by accessing it from a Web browser. Currently the queries are made on timestamps, which are used to determine the frequency with which PDUs are to be sent. But any possible queries can be made on the database to retrieve any information. The servlet can send the PDUs either in DIS mode or in HLA mode.



In our Pragmatic Object Web approach, we integrate CORBA, Java, COM and WOM based distributed object technologies. We view

Figure 5-8. Mak Stealth visualization for parallel CMS simulation of a heavy breach operation through a minefield in the Fort Knox terrain

CORBA and Java as most adequate for the middleware and back-end, whereas COM as the leading candidate for interactive front-ends due to the Microsoft dominance on the desktop market. Of particular interest for the M&S community seems to be the COM package called DirectX which offers a multimedia API for developing powerful graphics, sound and network play applications, based on a consistent interface to devices across different hardware platforms.

Using DirectX/Direct3X technology, we constructed a real-time battlefield visualizer, SimVis, that can operate both in the DIS and HLA modes. SimVis is a Windows NT application written in Visual C++ and the DirectX/Direct3D API. The ModSAF terrain is the input for a sampler program, which provides vertices, colors, and texture information for each of the faces. After the terrain is constructed, it is added as a visual object to the scenario scene. Geometry objects and animation sets for typical battlefield entities such as armored vehicles (tanks) and visual events such as explosions were developed using the 3D Studio MAX

authoring system. SimVis visual interactive controls include base navigation support, choice of rendering modes, and a variety of scene views.

The components described above have been combined into a demonstration that features an HPC parallel application (CMS) interacting with other simulation components running on geographically distributed computing resources. A typical configuration involves a parallel CMS federate running on Origin2000s at CEWES and ARL MSRCs and other modules (ModSAF; JDIS, the Java-based DIS/HLA bridge; PDUDB; SimVis) running on Syracuse SGI and NT workstations.

Our initial results are quite encouraging and we therefore believe that WebHLA with evolve towards a powerful modeling and simulation framework, capable of addressing new challenges of DoD and commodity computing in many areas that require federation of multiple resources and collaborative Web-based access such as Simulation Based Design and Acquisition.

5.5.2 WebFlow Activities

The value of high performance commodity computing (HPcc) is not limited to those applications requiring HLA compatibility. It is a new type of infrastructure that gives the user access to a full range of commercial capabilities (i.e. databases, compute servers), pervasive access from all platforms, and a natural incremental path for enhancement as the computer industry juggernaut continues to deliver software systems of rapidly increasing power.

The WebFlow system, which also underlies the WebHLA system described above,

is an HPcc system designed to provide seamless access to remote resources through the use of a CORBA-based middleware. During Year 3, Syracuse researchers have worked on using this tool to help couple together existing applications code and provide them with Web-based user interfaces in such a way that the user interface can run locally to the user, perhaps in the field, while the applications run on one or more "back-end" computational resources elsewhere on the network.



Figure 5-9. WebFlow Java client interface to access remote resources

The principal example developed during the year is the Land Management System (LMS), the development of which is lead by CEWES. The primary computational codes in LMS are EDYS, which simulates vegetation growth including disturbances (such as military exercises), and CASC2D, which simulates watersheds and the effects of rainfall. They interact with a third module, the Watershed Management System (WMS), which provides input processing and output visualization services to both codes. WMS requires a variety of input information including digital elevation models, land use data, and details of the soils and vegetation.

Once the user defines the simulation boundaries, the WebFlow system is used to extract the relevant information from databases, both locally, and Internet-accessible databases run by, for example, the U.S. Geological Survey. WMS processes the database extracts into input files appropriate for EDYS and CASC2D, and WebFlow then launches the simulation. Because of the construction of the simulation codes, CASC2D is invoked just once for the duration of the simulation and "paused" while the vegetation simulation is being run, while EDYS is invoked anew for each segment of the simulation. This, along with interconnection of the data streams for the two codes, is handled by WebFlow. It is also worth noting that the two codes happen to be run on separate platforms, in accord with their separate resource requirements. When the simulation is complete, WMS can be used through the Web-based interface to visualize the results.

The culmination of this project was a class, conducted by Tom Haupt at the CEWES MSRC, which discussed the tools and technologies used here and how they can be applied to other problems. This is yet another highly successful demonstration of the value and generality of the HPcc approach, and we look forward to helping users make further use of this software development model.

5.6 C/C: Collaboration and Communications (NPAC - Syracuse)

NPAC's efforts in the C/C area as a part of the CEWES MSRC PET effort encompass not just Collaboration and Communication, per se, but also the closely related area of tools and technologies for training and education. The NPAC team is also involved in analogous support activities in the ARL MSRC and ASC MSRC PET programs, as well as having a modest involvement in distance training and education activities in conjunction with the NAVO MSRC PET program. These additional connections provide a great deal of synergy with C/C activities sponsored by the CEWES MSRC.

The focus of our work has been understanding the needs and requirements for "collaboration and training" tools in the context of PET activities and to work towards their deployment. In this sense, we are strongly involved with both the rest of the PET team and the MSRC user community. At CEWES MSRC, our work has focused primarily on support for electronic training, and especially on synchronous tools for collaboration and training — support for "live" two-way interactions over the network. When combined with our activities for the other PET programs, this work becomes part of a unified whole, covering both synchronous and asynchronous tools for information dissemination, collaboration, and training.

This and other work at CEWES MSRC, combined with related activities at the other MSRCs in the collaboration and training area, have led us to develop an integrated picture of the current state of the art in both synchronous and asynchronous collaboration technology and how we believe they can be used effectively within the context of the PET program.

5.6.1 TANGO Interactive: Distance Training and Collaboration

During Years 2 and 3, NPAC has worked extensively with PET partner Jackson State University (JSU) on experiments in network-based distance education. Using NPAC's TANGO Interactive collaboratory framework, a series of semester-length academic credit (at JSU) courses have been taught by Syracuse-based instructors to students at JSU. The experience gained from these efforts has been critical in understanding both the technical and sociological factors surrounding distance education.

TANGO Interactive is a framework that allows sharing of applications across the Internet. It includes a suite of tools useful for basic collaboration and distance learning activities: shared Web browser, chat, whiteboard, audio/video conferencing, shared text editor, etc. It also provides an application program interface (API) that allows other applications to be hooked into the TANGO framework.

Tools of this sort are relatively new, and even the most computer-savvy have little or no experience with them. Consequently, it became clear rather early on that for these tools to gain acceptance in either collaborative or educational applications, they must be deployed in a staged fashion, starting from well-structured environments (i.e. classroom style educational use) and working towards less structured environments (i.e. general research collaboration).

During Year 3, NPAC collaborated with the Ohio Supercomputer Center (OSC), another CEWES MSRC PET partner, to transition the tools and experience from the JSU education efforts into the PET training arena. OSC provided instructors and course content, while NPAC worked with OSC, CEWES MSRC, and other recipient centers to provide support for the delivery tools (TANGO Interactive). This effort



Figure 5-10. Remote users participating in a Tango training class taught at the CEWES MSRC

expanded our experience to include instructors previously unfamiliar with the delivery tools, and while retaining the structured instructor/student relationship, the compressed delivery (over a few days rather than many weeks) introduced additional requirements on the robustness of the system.

This highly successful effort has led the way to what will become widespread and fairly routine use of distance training across the PET program in the coming year. It has also led to an increased interest in the use of the TANGO collaboratory in less structured environments, such as some kinds of meetings and research collaborations. This has given us a number of exploratory groups to work with as we begin the staged deployment of network collaboration tools into these progressively less structured situations.

5.7 SPP Tools: Scalable Parallel Programming Tools (CRPC – Rice and ICL - Tennessee)

The primary goal of SPP Tools in the CEWES MSRC PET effort is to promote a uniform, high-level, easy-to-use environment for programming available to all CEWES MSRC users and, ultimately, to all of DOD. We view "programming" very broadly, encompassing any means of describing a sequence of executable actions. This includes writing traditional CFD simulations as well as developing quick-and-dirty filters to scan output files. Similarly, we view "tools" as including any software that eases the task of programming. This includes tools, such as compilers, that make programming possible at all; it includes other tools, such as libraries, that provide easier-to-use facilities for programming; and it includes some tools, such as performance profilers, that help users understand their programs. SPP Tools thus cuts across disciplines.

If we are successful, all CTAs will benefit from the new tools. This has a long-term goal that will not be met by PET activities alone. In order to provide a complete set of tools, new resources will be needed. We therefore put great emphasis on collaboration with CEWES MSRC users (to understand the requirements for new tools), with other PET team members (to disseminate and test the tools), and with groups outside of DOD (to identify and develop the tools).

Year 3 project work of Rice included: Scalar Optimization for the CFD code HELIX; Use of OpenMP in HELIX; and an evaluation of CAPTools — a tool suite used for the upgrade or development of parallel application codes. These projects are summarized in the Appendix, and more detail appears in CEWES MSRC PET technical reports.

The Tennessee Year 3 SPP Tools effort focused on meeting the programming tool needs of a variety of DoD application developers and CEWES MSRC users, including those associated with code migration projects, CHSSI and DoD Challenge projects, and an SC98 HPC Challenge entry. Our approach has been to ensure that appropriate tools are installed and working properly on CEWES MSRC systems, to make information about installed tools available to as wide an audience as possible, and to provide one-on-one assistance to users as needed. All computational technology areas require robust, easy-to-use debugging and performance analysis tools. Since many DoD users develop and/or run applications on multiple MSRC platforms, it is highly desirable to have the same tools available across platforms so that users receive the maximum benefit from the time spent in learning to use a tool. Large-scale DoD applications often push tool capabilities to their limits, revealing scalability limitations and sometimes even breaking the tools. Thus, a major focus of our Year 3 effort was to provide users with reliable, effective cross-platform debugging and performance analysis tools and to work with tool developers and vendors to address scalability limitations of current tool technology.

5.7.1 HELIX: Scalar Optimization (Rice)

The Scalar Optimization project had significant merit. This project's findings resulted in the HELIX code being at least twice as fast, with no other changes required. The code was transformed from its original form to an equivalent form such that compiler optimization is effective. The key idea is to use intermediate scalar stores. This allowed the back-end code to use internal or working registers for intermediate storage. This technique reduced the latency costs associated with storing in ordinary memory, allowing temporary stores to occur in the high-speed registers. Thus, we recommend the technique to CEWES MSRC users.

5.7.2 HELIX: OpenMP (Rice)

The OpenMP Evaluation project was undertaken to investigate the efficacy of using OpenMP on production codes. Several small, synthetic benchmark codes were parallelized with OpenMP directives and demonstrated good decreases in overall execution time. Because of the favorable results from the Scalar Optimization project on the HELIX code, it was decided to attempt using OpenMP within this code. The HELIX code was profiled to find where the time is spent. More than 94% occurs in a single routine. This routine was a likely candidate to benefit by installing OpenMP directives, and using related compiler options and environment variables, at run time. However, only a modest speed up resulted. Upon further analysis of the HELIX code, it was found that the target routine performed small amounts of work each time it was called, but that the routine was called many times throughout the course of execution. This accounted for the overwhelming amount of overall time being spent with this routine, yet prevented effective parallelization with OpenMP. Our results demonstrate that OpenMP can be a simple and effective means to reduce execution time for some codes, but there exist codes for which OpenMP is not a suitable method of parallelization.

5.7.3 CAPTools (Rice)

Programming with CAPTools involved feeding the sequential implementation of a model nonlinear 2D elliptic PDE code to the CAPTools interactive parallelization system, and guiding the source-to-source code transformation by responding to various queries about quantities available only at runtime. An important issue with this software involves a significant licensing fee, thus limiting its availability to a few machines at CEWES MSRC. Results representative of "the state of the practice" for a scaled sequence of structured grid problems were given on three of the most important contemporary high-performance platforms: the IBM SP, the SGI Origin 2000, and the CRAY T3E.

5.7.4 Web-based SPP Tools Repository (Tennessee)

To enable CEWES MSRC users to find out about and learn to use appropriate tools, we have put together a Web-based Scalable Parallel Programming (SPP) Tools repository at: http://www.nhse.org/rib/repositories/cewes_spp_tools/catalog/

This repository contains a listing of tools being made available and/or being supported as part of our PET efforts. In addition to debugging and performance analysis tools, information is available about high performance math libraries, parallel languages and compilers, and parallel I/O systems. The repository includes a software deployment matrix that provides a concise view of which tools are installed on which platforms. By clicking on an entry for a particular tool and

a particular platform, the user can access site-specific usage information and tips as well as Web-based tutorials and quick-start guides.

The Repository in a Box (RIB) toolkit that was used to create the SPP Tools repository is available for CTAs and other PET support areas to use to make their software and tools more accessible and useful to users.

Debuggers listed in the SPP Tools repository include the cross-platform TotalView multi-process and multi-thread debugger, as well as platform-specific debuggers. Although we highly recommend TotalView, since it has excellent capabilities and is available on all CEWES MSRC platforms, information is included about platform-specific debuggers in case their special features are needed. Performance analysis tools listed include the Vampir cross-platform performance analysis tool, as well as platform-specific tools. We have worked closely with CEWES MSRC systems staff to ensure that the tools are properly installed and tested on CEWES MSRC platforms and to report any bugs to the tool developers.

5.7.5 CGWAVE: MPI_Connect (Tennessee)

For the SC98 HPC Challenge entry from CEWES involving the CGWAVE harbor response simulation code, we worked closely with the CEWES MSRC team to develop and debug a tool called MPI_Connect for MPI intercommunication between application components running on different machines at different MSRCs, so as to achieve multiple levels of parallelism and help reduce the runtime for CGWAVE from months to days. The MPI_Connect system is being made available for general use by DoD users who have similar intercommunication and metacomputing needs.

Springfield Frankford City St. Louis Nashyille Nashyille Memphis Montgomery On Rouge New Orleans New Orleans

Figure 5-11. Sites linked by MPI_Connect during the SC98 HPC Challenge computation

5.7.6 Virtual Reality Immersion for Performance Analysis: Virtue and Vampir (Tennessee)

Developers of several large-scale DoD applications — for example, the Mach 3 code used in the Radio Frequency Weapons DoD Challenge project at AF Phillips Lab — have run into scalability problems when trying to use current performance analysis tools technology. Trace-based techniques can produce extremely large and unwieldy trace files, which are difficult or impossible to store, transfer, and

analyze. For long-running simulations, it is often desirable to turn tracing on and off during execution, or to decide what further performance data to collect based on an analysis of data already collected during the same run. To address these issues, we are experimenting with dynamic instrumentation techniques and with virtual reality immersion to enable scalable performance analysis of large DoD applications. Using dynamic instrumentation, the user can monitor application execution during runtime, decide what data to collect, and turn data collection on and off as desired. We are initially using dynamic instrumentation to turn Vampir tracing on and off under user control, and to dynamically select, start, and read the values of hardware performance counters.

To address the problem of scalable visualization of large trace files, we have begun experimenting with 3D virtual reality immersion using the Virtue system developed at the University of Illinois. By using Virtue on an Immersadesk or a graphics workstation, the user can view state changes and communication behavior for the tasks making up a parallel execution in the form of a 3D time tunnel display that can be interactively manipulated and explored. The dynamic call tree for a process can be viewed as a 3D tree with sizes and colors of nodes representing attributes such as duration and number of calls. The amount of data that can be visualized at one time using 3D virtual immersion is an order or two of magnitude more than with a 2D display.

Virtue also has multimedia tools that allow remote collaborators to view and manipulate the same Virtue display (although scaled down and with fewer navigation capabilities) from their desktop workstations. We have successfully installed Virtue on the CEWES MSRC Scientific Visualization Lab systems. We have written a converter program that translates Vampir trace files into the data format understood by Virtue, and we have begun experimenting with Virtue to display large Vampir trace files produced by CEWES MSRC applications.

Our next step will be to enable scalable real-time performance visualization by linking dynamic instrumentation with Virtue. Performance data captured in real-time will be sent to the Virtue system where the user will be able to visualize the data. Our long-range goal is to allow the user to interact with and modify, or steer, a running application through the Virtue/dynamic instrumentation interface.

5.8 SV: Scientific Visualization (NCSA - Illinois, with ERC - Mississippi State)

During Year 3, we continued an active dialog with CEWES MSRC users and visualization staff, provided information about emerging developments in graphics

and visualization technology, transferred several tools into CEWES MSRC, assisted with visualization production, and conducted a training session.

As part of our technology watch efforts, we monitored the industry for new developments, paying particular attention to the rapidly increasing graphics capabilities of desktop PCs. We summarized these efforts in our annual "Report from SIGGRAPH" publication. We also canvassed users to assess their current data management strategies, and provided information discussing the applicability of NCSA's HDF5 data management package to CEWES MSRC users.

These activities are consistent with the 5-Year Strategic Plan developed for CEWES MSRC PET visualization:

http://www.wes.hpc.mil/CEWES/ctas/sv

This plan calls for initiatives in the following:

- Evaluating and extending co-processing environments.
- *Identifying strategies for management of very large datasets.*
- Defining user requirements for collaborative visualization.

Several application-specific tools were transferred to CEWES MSRC users, and training was provided in their use. These tools include CbayVisGen, CbayTransport, ISTV and DIVA, and volDG. These tools are having direct impact on CEWES MSRC users' ability to do their work.

5.8.1 CbayVisGen and CbayTransport (NCSA): EQM

CbayVisGen is a visualization tool specially designed to support the visualization needs of Carl Cerco and his EQM team at CEWES. This group is investigating long-term phenomena in Chesapeake Bay, with results being provided to the EPA. CbayVisGen used existing visualization libraries and customized a tool to visualize the hydrodynamics and nutrient transport activity over 10-year and 20-year time periods. Cerco's work has moved to full production runs, and he has frequent needs to share his results with his EPA science monitor. Therefore, CbayVisGen was customized to include easy image and movie capture, which can be easily transferred to a Web page for sharing with his colleagues. A follow-on tool, CbayTransport, experimented with alternatives for visualizing the transport flux data. Cerco had no mechanisms for viewing this part of his data, so this tool has added new and needed capability.

5.8.2 DIVA and ISTV (MSU): CWO

The DIVA and ISTV visualization tools, developed at MSU's ERC, supported visualization for the CWO user community of CEWES MSRC. Both tools were put to an initial task of generating stills and movies, in an effort to assess applicability of each tool. Later, ISTV was chosen to visualize the output of a CH3D model of the lower Mississippi River. We have also used ISTV to show WAM output. Robert Jensen of CEWES reports

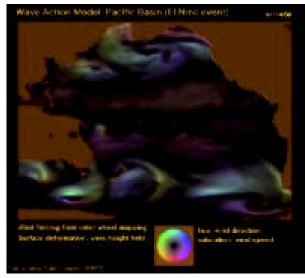


Figure 5-12 WAM visualization of the El Nino event in the Pacific Basin

that ISTV has been useful for looking at correlations between variables. Animating through the time-series with ISTV was especially revealing — a throbbing effect is seen, apparently due to the assimilation of wind data every 3 hours. The significance of this is currently under study. Finally, ISTV is used to look at the coupled WAM-CH3D model being tested. We anticipate that continued use of these tools in varied applications will further understanding for the warfighter of the forces encountered during littoral operations.

5.8.3 voIDG (MSU): CSM

The visualization tool volDG from MSU was designed to explore the use of wavelet representations for very large datasets. Wavelet representation provides a compression scheme useful for large data. Wavelets can also support detection of features, such as singularities, which can guide meaningful access and transfer of very large datasets. For example, structure-significant encoding of a dataset is possible. In subsequent data exploration, regions of high significance can be examined first.

5.8.4 Computational Monitoring and Interactive Steering (NCSA): EQM

The PET SV team also conducted an in-depth review of the various software packages available to support computational monitoring and interactive steering. In our initial report, we summarized the characteristics of several of these tools. We also applied the most promising of these tools to a CEWES MSRC

application, the parallel version of CE-QUAL-ICM, and reported on this hands-on activity. In conjunction with this effort, we connected the CE-QUAL-ICM code to NCSA's Collaborative Data Analysis Toolsuite (CDAT). CDAT is a multi-platform collection of collaborative visualization tools. In this scenario, participants on an ImmersaDesk, a desktop workstation, and a laptop were able to simultaneously explore the simulation output as it was generated from a 12-processor run of CE-QUAL-ICM. This was a particularly rewarding effort, because it involved staff from across the PET team. The parallel version of CE-QUAL-ICM is the work of Mary Wheeler's (Texas) EQM PET team. NCSA was responsible for the visualization tools. Those tools derive their collaboration capabilities from TANGO Interactive, from Geoffrey Fox's C/C team (Syracuse) in CEWES MSRC PET.

5.9 USC HPC Benchmarking

Although many High Performance Computing (HPC) platforms have been deployed at various MSRCs, there has been a "gap" in understanding the underlying architecture from an end-user's perspective. To further complicate matters, operating system characteristics, compiler features, and various standards affect the performance of user applications. Most MSRC end-users have been developing their applications ad hoc without much consideration given to the performance of their algorithms. The goal of the USC team's focused effort was to develop a set of benchmarks and a model of the underlying architecture in order to help end-users develop efficient parallel algorithms for their applications.

To evaluate the performance of HPC platforms deployed at the MSRCs, researchers have proposed various benchmarks. Some benchmarks attempt to measure the peak performance of these platforms. They employ various optimizations and performance tuning to deliver close-to-peak performance. These benchmarks showcase the full capability of the products. However, for most users these performance measures seem to be meaningless. For end-users, the actual performance depends on a number of factors including the architecture and the compiler used. Other benchmarks attempt to measure the performance of these platforms with a set of representative algorithms for a particular scientific domain. Although useful, these benchmarks do not give the end-users a simple method for evaluating their algorithms and implementations.

The USC team has taken a novel approach to benchmarking that addresses the actual performance available to end-users. The benchmarks allow the end-users to understand the machine characteristics, the communication environment, and the compiler features of the underlying HPC platform at a user level. Using the results of these benchmarks, the USC team is able to provide end-users with a

simple and accurate model of HPC platforms, including that of the software environment. Using such a model, end-users can analyze and predict the performance of a given algorithm. This allows algorithm designers to understand tradeoffs and make critical decisions to optimize their code on a given HPC platform.

Distributed Memory Systems such as the IBM SP and Shared Memory Systems such as the SGI/CRAY Origin2000 are widely used HPC platforms. Some hybrid systems such as the SGI/CRAY T3E attempt to provide features of both types of architectures by including message passing capabilities and a globally shared address space. In using these HPC platforms, there are several layers of interface to the actual hardware. These include the operating system, compilers, library codes for computation and communication such as ScaLAPACK, PBLAS, MPI, etc, and other support utilities. Initially the USC team investigated all the various features that affect the performance for end-users and formulated a set of parameters to model these factors.

In order to measure these parameters, a large set of experiments was conducted on all available platforms. The results were then carefully evaluated to produce a coherent picture of the factors affecting the performance of the HPC platforms. From these analyses, the USC team determined that in predicting the performance of algorithms on HPC platforms, the key factor is an accurate cost analysis of data access. The cost for communication of data is heavily affected by the data location. The data may be physically located in the local memory, in a remote processor, or on secondary storage such as a disk. The various possible data locations can be thought of as a data hierarchy. Thus, data may be communicated between processor and memory, between processors or between secondary storage and the processor. The cost to access data increases dramatically as the data moves down along the hierarchy. The USC team's benchmarks measure the cost of accessing the data along this hierarchy.

From these benchmark results, the USC team has generated a set of parameters and formulated the Integrated Memory Hierarchy (IMH) model. The IMH model provides a uniform set of parameters across multiple platforms that measures the cost of communication from various levels of the data hierarchy. This allows end-users to evaluate and predict the performance of their algorithms on a particular HPC platform.

In order to evaluate the benchmark results and the IMH model, the USC team has optimized a CFD application supplied by an end-user. A detailed explanation of this optimization is included in Section 8 on outreach to users. This optimization effort resulted in a win-win situation for the end-user as well as for the USC team.

The optimization efforts produced an algorithm with approximately a 5-fold increase in performance using 30 processors compared with the original algorithm. The resulting optimized algorithm remained scalable well beyond 30 processors and was only limited by the size of the data to be processed.

The benchmark results and the IMH model allow end-users to evaluate and predict the performance of their algorithms on a particular HPC platform. A uniform set of parameters across multiple platforms allows end-users to make intelligent decisions in selecting the best platform for a given application. Once a platform has been selected, the end-user can use the IMH model to evaluate the performance of their algorithm. Using this evaluation in conjunction with the developed optimization techniques, they can modify and optimize their code to achieve superior performance. The end-user will also be able to estimate the performance of various algorithm alternatives without actual coding, thus greatly reducing the time for developing optimized applications.

This page intentionally left blank

6. TOOLS INTRODUCED into CEWES MSRC

The enhancement of the programming environment at CEWES MSRC through the identification and introduction of programming tools, computational tools, visualization tools, and collaboration/communication tools is a major emphasis of the CEWES MSRC PET effort. Tools introduced into CEWES MSRC by the PET team during Year 3 are listed in Table 4. The CEWES MSRC PET team has provided training courses at the CEWES MSRC and at remote user sites for many of these tools (see Section 7), and continually provides guidance and assistance in their use through the on-site team. The purpose of this present section is to discuss the function of these tools and their importance to CEWES MSRC users. Many of these tools came from collaborative efforts across various components of the CEWES MSRC PET team, both on-site and at the universities.

6.1 Programming Tools

An ongoing evaluation of the state-of-the-art in parallel debuggers and performance analysis tools is carried out by the PET SPP Tools team at Tennessee, as part of the National HPCC Software Exchange (NHSE) effort. From these findings Tennessee is able to recommend, install, test, and evaluate the utility of such tools within the CEWES MSRC user community. At present, five parallel performance analysis tools (Vampir, MPE Logging Library and nupshot, AIMS, SvPablo, and ParaDyn) and one debugger (Totalview) have been made available to CEWES MSRC users on appropriate platforms.

Performance analysis tools typically require the addition of code to a program (known as instrumentation) in order to output trace information to a file that will later be interpreted and displayed with a GUI interface. Their purpose is to document significant events (e.g., subroutine calls, sending or receiving messages, I/O, etc) within the execution of the user's code. Debuggers allow a programmer to examine codes as they execute in an attempt to determine the cause of and to then fix catastrophic errors.

6.1.1 TotalView

TotalView is a multi-process and multi-thread, source level debugger with a graphical user interface. Versions are available for all CEWES MSRC platforms.

Tennessee evaluated and recommended buying TotalView. Tennessee has worked with CEWES MSRC systems staff to get TotalView properly installed and integrated with the queuing system. Tennessee has provided site-specific usage information, training, and a Web-based tutorial for TotalView. Tennessee served

as a beta-tester for new releases of TotalView, tested the CEWES MSRC Totalview installations, and reported bugs to the TotalView developer.

Being able to quickly learn and start using a full-featured parallel debugger that works properly in the CEWES MSRC environment has enabled the MSRC Computational Migration Group (CMG) to understand the execution of parallel codes and find and fix elusive bugs. For example, TotalView was used to isolate Cray pointer bugs in a code called MSPHERE that would have been difficult to find without TotalView. Having a single debugger that works across platforms has given CEWES MSRC users a higher payoff for the time invested in learning the debugger and has enabled the CMG to more effectively support users in their debugging tasks.

6.1.2 Vampir

Vampir is a performance analysis tool for MPI parallel programs. Vampir consists of two parts — the Vampirtrace library that can be linked with an application to produce a trace file during program execution, and the Vampir visualization tools for analyzing the resulting tracefile. Pallas, the developer of Vampir, is working with OpenMP compiler vendors to develop Vampir support for tracing and visualizing execution of OpenMP applications. Users will be allowed to mix MPI and OpenMP, as long as the MPI implementation is sufficiently thread-safe.

Tennessee has evaluated Vampir, recommended purchase, and made suggestions for improvements to Vampir 1.0 that were implemented in Vampir 2.0. Tennessee has provided site-specific usage information, training, a Web-based tutorial, and user assistance for Vampir.

Having a robust performance analysis tool that works across platforms has enabled CEWES MSRC users to quickly and easily collect performance trace data and analyze that data visually to spot communication bottlenecks in their codes. Vampir has been used by CEWES MSRC user David Rhodes to analyze and improve performance of the CEN-1 Harmonic Balance Simulation code. Vampir has been used by the RF Weapons Challenge team of AF Phillips Lab to achieve a significant performance improvement in the ICEPIC code.

6.1.3 MPI_Connect.

MPI_Connect, a communication system developed at Tennessee, enables multiple HPC systems to be used effectively on the same MPI application, thus enabling larger problems to be solved more quickly. The capability of using tuned vendor MPI implementations with small overhead permits highly efficient communication within a single system. Together with OpenMP and MPI, MPI_Connect has been

used to reduce the runtime required for the CGWAVE harbor response simulation code of CEWES from months to days. This project won the Most Effective Engineering Methodology award for its SC98 HPC Challenge entry.

MPI_Connect is being made available to other CEWES MSRC users and application developers who have similar application coupling and metacomputing needs.

6.1.4 Virtue

The University of Illinois developed the Virtue system for visualization and analysis of performance data using virtual reality immersion. In the CEWES MSRC PET effort, Tennessee has written a vampir2virtue converter and is working with Illinois to implement additional features in Virtue that will provide more effective visualization of parallel programs (e.g., better labeling of Virtueobjects).

Virtue will enable effective visualization of the execution of large-scale applications through the use of 3D and immersive virtual reality, thus enabling performance bottlenecks to be found and fixed more easily. Virtue can be used with the Immersadesk or with graphics workstations. Virtue has multimedia tools that allow remote collaborators to view and manipulate scaled-down versions of Virtue displays from their desktop workstations and interact using voice and video.

6.1.5 PAPI

With input from users, researchers, and vendors, Tennessee has written a specification for a portable API, called PAPI, for accessing hardware performance counters. Tennessee is currently working on reference implementations of PAPI for the SGI/CRAY Origin2000 and Linux, with an IBM SP implementation planned for the near future.

The PAPI portable interface to hardware performance counters will enable CEWES MSRC users to use the same set of routines to access comparable performance data across platforms. Hardware performance counters can provide valuable information for tuning the cache and memory performance of applications. PAPI will also enable CHSSI code developers to more quickly and easily obtain data needed for performance reporting requirements.

6.1.6 dyninst

The University of Maryland has produced the dyninst library, which provides an API for attaching to and instrumenting an executable, running on a single process.

In the CEWES MSRC PET effort, Tennessee has tested dyninst on the Tennessee IBM SP and is currently testing on the CEWES MSRC IBM SP (pandion). After testing, plans are to install dyninst as unsupported software and to provide site-specific usage information. Dyninst will enable users to attach to a running application and monitor or even change application behavior dynamically.

6.1.7 DPCL

The Dynamic Probe Class Library (DPCL) is a client-server extension of dyninst that has been developed by IBM for use with parallel and distributed applications. IBM has provided Tennessee with a beta release of DPCL for the IBM SP and with the DPCL source code. Tennessee will test DPCL on the CEWES MSRC IBM SP (pandion) and will port DPCL to the Origin2000. Tennessee will develop some demonstration end-user tools on top of DPCL and will provide site-specific usage information.

DPCL will provide a cross-platform infrastructure for runtime application instrumentation for the purposes of performance analysis, computational steering, and data visualization. DPCL can be used directly by users but also by developers of end-user tools. For example, DPCL will be used to enable Vampir tracing to be turned on and off at runtime and to enable runtime selection and control of access to hardware performance counters. The DPCL infrastructure reduces the amount of effort needed to develop new tools, allowing end-users to develop their own special-purpose tools quickly and easily.

6.1.8 Repository in a Box (RIB)

RIB is a toolkit developed at Tennessee for setting up and maintaining an interoperable, distributed collection of software repositories.

RIB provides an easy-to-use interface for PET CTA on-site leads to enter and maintain information about software being made available to CEWES MSRC users as a result of PET and CHSSI efforts. RIB's interoperation capabilities allow software cataloging done at one site to easily be made available to other sites and allows virtual views of a distributed collection of repositories to be created. The software deployment feature of RIB allows users to quickly access information about what software is available on what MSRC machines and about how to use the software. So far, RIB has been used to establish CEWES MSRC repositories for SPP Tools, CFD, and grid generation software.

6.1.9 CAPTools

The Computer Aided Parallelization Tools (CAPTools) is a semi-automatic tool to assist in the process of parallelizing Fortran codes. This tool is under development at the University of Greenwich. The main components of the tools comprise:

- A detailed control and dependence analysis of the source code, including the acquisition and embedding of user supplied knowledge.
- User definition of the parallelization strategy.
- Implementation.
- Automatic migration, merger, and generation of all required communications.
- Code optimization including loop interchange, loop splitting, and communication/calculation overlap.

To run a CAPTools generated code, users need to link the compiled code with the CAP library.

6.2 Previously-Evaluated Tools

The following lists programming tools previously evaluated and made available as appropriate at CEWES MSRC.

6.2.1 nupshot

nupshot is a trace visualization tool that has a very simple, easy-to-use interface and gives users a quick overview of the message-passing behavior and performance of its application. nupshot analyzes trace files that are produced by the MPE Logging Library. Both nupshot and the MPE Logging Library were originally designed as extensions of MPICH from Argonne and MSU. Tennessee made minor modifications to the MPE Logging Library so that it will work with the native MPI libraries on the IBM SP and SGI Origin2000.

6.2.2 AIMS

AIMS is a freely available, trace-based performance analysis tool developed by the NASA Ames NAS Division that provides flexible automatic instrumentation, monitoring, and performance analysis of Fortran 77 and ASCI message-passing applications that use MPI or PVM.

6.2.3 SyPablo

SvPablo, another trace-based performance analysis tool, has a GUI that lets the user determine which portions of the source code are selected for instrumentation and then automatically produces the instrumented source code. After the code executes and a trace file has been produced, the SvPablo GUI displays the resulting performance data alongside the source code. SvPablo runs on Sun Solaris and SGI workstations and on the SGI Origin2000. It can access and report results from the MIPS R10000 hardware performance counters on the SGI Origin2000.

6.2.4 ParaDyn

ParaDyn is designed to provide a performance measurement tool that scales to long-running programs on large parallel and distributed systems. Unlike the other tools that do post-mortem analysis of trace files, ParaDyn does interactive runtime analysis.

6.2.5 MPE Graphics Library

The MPE Graphics Library is part of the MPICH package distributed by Argonne National Laboratory. This graphics library gives the MPI programmer an easy-to-use, minimal set of routines that can asynchronously draw color graphics to an X window during the course of a numerical simulation. A user can use the graphics routines to scrutinize the execution of a code with respect to monitoring the accuracy and progress of the solution or as a debugging aid.

6.2.6 ScaLAPACK

ScaLAPACK is a library of routines for the solution of dense, banded and tri-diagonal linear systems of equations and other numerical linear algebra computations. Data sharing between distributed processors is accomplished using the Basic Linear Algebra Communication Subroutines (BLACS).

6.2.7 PETSc

The Portable, Extensible Toolkit for Scientific Computation (PETSc) is a suite of data structures and routines for the solution of large-scale scientific application problems modeled by partial differential equations. PETSc was developed within an object-oriented framework and is fully usable from Fortran, C and C++ codes.

	Robustness/ Accuracy	Usability	Portability	Scalability	Versatility
AIMS	Fair	Good	Fair	Good	Good
nupshot	Good	Good	Good	Good	Good
Pablo Analysis GUI	Good	Fair	Fair	Good	Excellent
Paradyn (MPI Version)	Fair	Good	Fair	Fair	Good
SvPablo	Good	Good	Fair	Good	Good
VAMPIR	Excellent	Good	Excellent	Excellent	Good

Figure 6-1. Evaluation of performance and debugging tools

6.3 Visualization Tools

Several visualization tools were introduced into the CEWES MSRC during Year 3. We conducted an in-depth survey of the software tools available for computational monitoring and interactive steering. These tools include CUMULVS (from Oak Ridge National Lab), DICE (from the Army Research Lab), pV3 (from MIT), and others. Computational monitoring tools can be very valuable for the MSRC user. On the one hand, visualizing intermediate results can identify a run that is not going well — the user can cancel the run without wasting their allocation. Further, computational monitoring is invaluable for debugging new codes, which is particularly useful as more teams move toward coupled models. Finally, for codes that produce very large datasets, computational monitoring might be the only practical way to view the simulation output. We experimented with using each of these tools applied to a CEWES MSRC code. Results from this study are provided in a CEWES MSRC PET Technical Report. We also conducted a one-day training session to introduce these tools. This has resulted in several follow-up contacts where CEWES MSRC users are interested in the benefits offered by applying these techniques to their codes.

6.3.1 CbayVisGen and CbayTransport

CbayVisGen was specially designed by the PET SV team at NCSA to support the visualization and collaboration needs of Carl Cerco and his EQM team at CEWES. This tool enables them to visualize the hydrodynamics and nutrient transport activity over 10-year and 20-year time periods of activity in

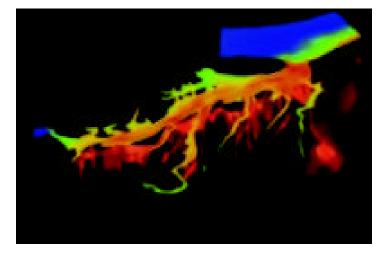


Figure 6-2. Visualization of dissolved oxygen in Chesapeake Bay

Chesapeake Bay. A follow-on tool, CbayTransport, experimented with alternatives for visualizing the transport flux data. Cerco had no mechanisms for viewing this part of his data, so this tool has added new and needed capability.

6.3.2 Collaborative Data Analysis Toolsuite (CDAT)

A prototype toolsuite for collaborative visualization was also introduced to CEWES MSRC by NCSA. The Collaborative Data Analysis Toolsuite (CDAT) is a multi-platform collection of collaborative visualization tools. Using components from this toolsuite, participants on an ImmersaDesk, a desktop workstation, and a laptop are able to simultaneously explore simulation output. Collaborative visualization is potentially very useful to CEWES MSRC users.

6.3.3 voIDG

The visualization tool volDG was introduced to Raju Namburu of CEWES to explore the usefulness of wavelet representations and structure-significant encoding of very large structures data. VolDG results from a GUI-based software project developed in collaboration between the ERC at Mississippi State and Mitsubishi Electric Research Laboratories.

This tool includes both volume rendering capabilities and an inverse design algorithm that allows for the search for structures in the data. The latter feature of this tool allows the user to be cognizant of the inherent features in the dataset, while the former feature allows preview of the volume in a semi-transparent mode. The impact of this tool is currently limited to the use of the first feature, namely

volume rendering. Since CSM datasets are composed of material interfaces, the use of semi-transparency can be useful in visualizing structures in a juxtaposed way. Such a tool can allow better understanding of the datasets. This is the first time such a capability has been provided to a CSM user at CEWES MSRC.

6.3.4 ISTV

The visualization tool ISTV from the ERC at Mississippi State was introduced to the CWO user community of CEWES MSRC. ISTV was used to visualize the output of a CH3D model of the lower Mississippi River and to show WAM output. Robert Jensen of CEWES reports that ISTV has been useful for looking at correlations between variables. Animating through the time-series with ISTV was especially revealing — a throbbing-effect is seen, apparently due to the assimilation of wind data every 3 hours. The significance of this is currently under study. These tools have potential for facilitating understanding of the forces encountered during littoral operations.

6.4 Communication/Collaboration Tools

6.4.1 TANGO Interactive

TANGO Interactive is a Java-based Web collaboratory developed by NPAC at Syracuse University (with initial funding from AF Rome Lab). It is implemented with standard Internet technologies and protocols, and runs inside an ordinary Netscape browser window (support for other browsers is in progress). TANGO delivers real-time multimedia content in an authentic two-way interactive format. TANGO was originally designed to support collaborative workgroups, though synchronous distance education and training, which can be thought of as a highly structured kind of collaboration, had become one of the key application areas of the system.

The primary TANGO window is called the Control Application (CA). From the CA, participants have access to many tools, including:

SharedBrowser, a special-purpose Web browser window that "pushes" Web documents onto remote client workstations.

- WebWisdom, a presentation environment for lectures, foilsets, and similar materials.
- Whiteboard, for interactive text and graphics display.
- Several different kinds of chat tools.

• BuenaVista, for two-way audio/video conferencing.

TANGO has been deployed for some time at the CEWES MSRC and at Jackson State University for use in joint Syracuse-Jackson State distance education work begun in Year 2. More recently, TANGO Interactive has been used to deliver PET training through installations at all four of the MSRCs and other sites as well.

During Year 3, a substantial investment of effort has been made in the TANGO Interactive system to increase its stability and robustness to a level commensurate with demands of routine use in education, training, and collaboration. These efforts resulted in the first release suitable for general deployment, in May 1998, and a new release with additional improvements at the end of Year 3.

6.5 Computational Tools

6.5.1 WebHLA

The WebHLA set of tools is being introduced into CEWES MSRC by NPAC at Syracuse in connection with PET support of the FMS CTA. WebHLA is a collection of tools, packaged as HLA federates and used for integrating Web/Commodity based, HLA compliant and HPC enabled distributed applications. WebHLA tools/federates, which are being completed now and to be transitioned to CEWES MSRC and ARL MSRC, include:

- JWORB (Java Web Object Request Broker) a universal middleware server written in Java that integrates HTTP, IIOP and DCE RPC protocols, i.e. it can act simultaneously as Web Server, CORBA broker and DCOM server.
- OWRTI (Object Web RTI) a Java CORBA implementation of DMSO RTI 1.3, packaged as JWORB service and used as a general purpose federation and collaboration layer of the WebHLA framework.
- JDIS a Java based DIS/HLA bridge that allows rapid conversion of legacy DIS applications to HLA federates so that they can play in any standard-compliant HLA federation environment.
- PDUDB a SQL/XML based support for simulation logger and playback; all DIS PDUs or the equivalent HLA interaction events are passed as XML messages to and recorded in an SQL database to be replayed later for training, demo or other analysis purposes.
- SimVis a commodity (Microsoft DirectX/Direct3D) based 3D real-time battlefield visualizer for DIS/HLA simulations.

6.5.2 CTH and EPIC Tools

Several software modules and programming tools have been developed by TICAM at Texas in CEWES MSRC PET support of the CSM CTA. These include the following:

- Software modules for error indicator computation in CTH.
- Software modules for error indicator computation in EPIC.
- Software to incorporate block refinement in parallel simulations for CTH.
- *Software to adaptively refine and update the data structure of EPIC.*
- Software for Morton/Hilbert space-filling curve generation.
- A Utility tool for code testing and validation.
- Software for advanced front tracking in CTH under adaptation.

Some of the software modules for error indicators are more broadly applicable (with perhaps minor modification) to other PET program analysis components. The software for adaptive refinement and data structure modification is more specific to the application codes in question but the concepts are general. The module for the Morton/Hilbert curves is written in C++ and has quite general applicability. The Utility tool approach can be applied to other applications and codes. The integrated effect of these developments on the CEWES MSRC is significant since it will provide a new adaptive analysis capability and spearhead similar extensions to the DoD application codes both in CSM and the other CTA areas.

6.5.3 Integrated Memory Hierarchy (IMH) Model

The Integrated Memory Hierarchy (IMH) Model, while not a conventional computer tool, is a simple and easy to use model of current HPC platforms available at MSRCs. The IMH model allows end-users to predict the cost of data movement from various levels of the memory hierarchy. This consists of communication between the processor and its memory, other processors, and secondary storage. The model integrates the impact of various architectural features, operating system characteristics, communication environment, and compiler features that the user interacts with in implementing an algorithm. The model consists of a uniform (over several platforms) set of key parameters that captures the performance of the underlying platform from a user's perspective.

Using the IMH Model, end-users can analyze and predict the performance of their algorithms for a particular HPC platform. This allows them to make intelligent trade-offs in their algorithm design without actual coding and to quickly develop optimized applications that are both scalable and portable across various HPC platforms.

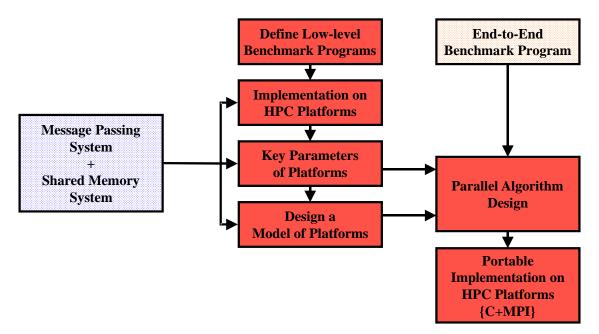


Figure 6-3. Model for the analysis of algorithms and code performance on HPC platforms

7. USER TRAINING

Since its inception, the CEWES MSRC PET training program has faced two challenges. One is to provide training in an anytime, any pace, any place environment. That goal has not been reached, but the PET program has continued to support efforts in remote training and distance education. Those efforts are now bearing fruit as can be seen from this report. The second challenge is to meet the needs of CEWES MSRC users faced with a rapid change in available hardware and software systems. The attempts to meet this challenge are evident by



Figure 7-1. MSU transmission equipment used in the satellite broadcast of the first HPCMP MSRC training class (1996)

comparing the courses listed in Table 7 with the list that appeared in the Year 2 Annual Report. Training is now offered on products like OpenMP that did not exist in 1997, and courses on topics such as C++ have been replaced by Java courses.

The PET training program continued its evolution in Year 3 with more emphasis on distance training technology and service to remote users. The first full-blown distance training course was offered through the TANGO Interactive distance collaboration system. This was followed by a second TANGO course that was broadcast to the other three MSRCs. This year has also seen continuous development of TANGO as a distance education tool through its application as a vehicle for offering graduate computer science courses from Syracuse University to Jackson State University, and now an undergraduate course from Jackson State to Morgan State.

The Fortran 90 course offered in September 1998 was our first TANGO-based course offered to remote users. The course was broadcast over the Internet to PET partner Ohio Supercomputer Center (OSC), the course provider, and users at the ARL MSRC. Additional TANGO courses have been scheduled for 1999.

The PET training team supports not only training activities, but also provides logistic and technical support to all areas of the PET program. PET played a major role in supporting the workshop on Recent Advances in Computational Structural Mechanics and High Performance Computing held at CEWES in November 1998.

7.1 Training Curriculum

PET training is designed to assist the CEWES MSRC user in transitioning to new programming environments and efficiently using the present and future SPP (Scalable Parallel Processing) hardware acquired under the HPCMP program. The training curriculum is a living document with new topics being added continually to keep up with the fast pace of research and development in the field of HPC. The curriculum contains courses in the following general categories:

Parallel programming.

Architecture and software specific topics.

Visualization and performance.

CTA targeted courses, workshops, and forums.

Table 7 gives a list of all training courses taught during Year 3 with the organization offering the course, the number of students attending the course, and the overall evaluation score of the course on a scale of 1 (poor) to 5 (excellent). Unless otherwise noted, the courses were held in the CEWES MSRC Training and Education Facility (TEF).

7.2 Training at the DoD HPCMP User Group Meeting

The CEWES MSRC PET program sponsored training activities at the DoD HPCMP Users Group Conference at Rice in June 1998. Five training courses were held and are included in the list of courses in Table 7. These training courses had the largest attendance in the history of the User Group Conferences.

The PET program also sponsored a PET Training Colloquium on Distance Learning and Collaboration. The colloquium was organized by Prof. Geoffrey Fox, PET Senior Academic Lead for Collaboration/Communication, from Syracuse University. The speakers were Dr. Anoop Gupta of Microsoft Research, Dr. Don Johnson of the DoD Advanced Distributed Learning Initiative, and Fox. The moderator was Dr. Louis Turcotte of CEWES MSRC.

7.3 Seminars

The CEWES MSRC PET program offers seminars on an irregular basis. These are presentations by experts in their field and are designed to introduce the CEWES MSRC users to current research topics in HPC. The following seminar presentations were made during Year 3 at CEWES MSRC:

Managing Scientific Data with HDFD Michael Folk National Center for Supercomputing Applications (NCSA)University of Illinois

Web-Based Instruction Prof. Geoffrey Fox Director, Northeast Parallel Architectures Center (NPAC) Syracuse University

7.4 Web-Based Training

During Year 3, two training classes were offered to remote users through TANGO. The Fortran 90 class on October 28, 1998 was received by users at ARL. Users at ARL, ASC, and NRL received the Origin2000 class taught on January 26-27, 1999. Both classes were taught in the CEWES MSRC TEF by instructors from OSC. Remote users were able to fully participate in the classes through the audio and video conferencing capabilities of TANGO. During the fall semester of 1998, the distance education course Computational Science for Simulation Applications, delivered to Jackson State from Syracuse via TANGO, was made available for audit in the TEF by CEWES MSRC users.

7.5 Training Course Descriptions

This material appears on the CEWES MSRC PET Web site as training course descriptions in advance of courses, hence the future tense.

7.5.1 Parallel Programming Workshop for Fortran Programmers

The workshop will begin with a one-day lecture on strategy, tools, and examples in parallel programming. On the remaining days participants will work with their own codes. There will be no attempt to prescribe a particular solution to the problem of porting a code from the C90 to the scalable systems. Rather, the instructors will work with the user to find the best overall strategy, whether that best strategy is message passing via MPI or PVM, or data parallel via HPF or OpenMP. It may not be possible to parallelize a full-blown application program in a week, but the process can get started and a continuing relationship can be established between the users and the parallelization experts at the CEWES MSRC.

7.5.2 Using the Message Passing Interface (MPI) Standard

Message Passing Interface (MPI) is the de facto standard for message passing developed by the Message Passing Interface Forum (MPIF). MPI provides many features needed to build portable, efficient, scalable, and heterogeneous message

passing code. These features include point-to-point and collective communication, support for data types, virtual topologies, process-group and communication context management, and language bindings for the FORTRAN and C languages. In this tutorial we will cover the important features supported by MPI with examples and illustrations. Also an introduction to extensions of MPI (MPI-2) and message passing in real-time (MPI/RT) will also be provided.

7.5.3 Large Deformation Computational Structural Mechanics Applications on High Performance Computers using ParaDyn/DYNA3D

This course began with a DYNA3D lecture reviewing the features added to the program since 1993. Some recent features include techniques for switching materials from rigid to deformable and back, new material models and equations of state, recent developments in element technology, and new contact methods. This lecture will include time for questions and answers about modeling and using any of the features in DYNA3D. The MSRC will provide attendees a summary of steps required for submitting batch jobs to run parallel problems on the Origin2000, CRAY T3E, and IBM SP. This will include the design of script files for the batch system, a discussion of the batch queues, and running the batch utilities to follow the progress of a job. The ParaDyn lecture will feature discussions on the automated software for domain decomposition, running the ParaDyn program, post-processing the results for visualization, and the performance on parallel computers. Techniques for efficiently handling contact boundary conditions and future parallel capability releases will be discussed. The lectures will finish with a discussion of applications illustrating the power of parallel computers in modeling problems of DoD interest. On the second day the instructor will demonstrate a sample problem preparation and execution of a ParaDyn calculation on one of the parallel systems at CEWES MSRC. Attendees will be able to run their own examples and work with the instructor directly at this time.

7.5.4 Grid Generation for Complex Configurations

This course will cover an in-depth review of the current state-of-the-art and state-of-practice in geometry/grid generation applicable to complex problems. A step-by-step process starting from the initial CAD definition or drawing of a configuration and proceeding to the generation of a curvilinear, hexahedral or cartesian grid and grid adaptation techniques will be presented in detail. Demonstrations and hands-on computer lab exercises will be conducted to explore the use of GUM-B, VGRID, CAGI, GENIE++, TrueGrid, PMAG, CUBIT, and Hybrid2d systems for practical applications of interest to CEWES MSRC users.

7.5.5 Java for Scientific Computing

The objective of this course was to provide the participant with the following:

An understanding of the high performance computing architecture, including the World Wide Web for visualization.

An overview of the Java language and its capabilities.

Enough programming details to do some examples.

7.5.6 High Performance Fortran (HPF) in Practice

This course introduced programmers to the most important features of HPF, including features inherited from Fortran 90, the data parallel FORALL statement and INDEPENDENT assertion, and data mapping by ALIGN and DISTRIBUTE directives. The instructor will illustrate how these features can be used in practice on algorithms for scientific computation such as LU decomposition and the conjugate gradient method.

7.5.7 Performance Optimization

This course will focus on the optimization of numeric intensive codes for HPC systems. The course will begin with a quick overview of the basics of performance and processor architecture. Then it will cover a wide variety of optimizations geared towards enhancing processor performance. Topics will include efficient use of the memory hierarchy, functional units, amortizing loop overhead and dependency analysis. Common bottlenecks and caveats will be discussed as well as proposed solutions, and the logic behind them.

7.5.8 Topics in Finite Element Methodology for Nonlinear Problems

This course is broadly structured to cover different types of applications from structures to fluids to heat transfer and coupled problems that are of general interest to DoD. Methodology, rather than specific applications, is stressed. Topics covered include algorithms, nonlinear solution strategies, and integrating solution with adaptive refinement.

7.5.9 A Tutorial on Designing and Building Parallel Programs

In this tutorial, the instructors will provide a comprehensive introduction to the techniques and tools used to write parallel programs. First, the instructors will introduce principles of parallel program design, touching upon relevant topics in architecture, algorithms, and performance modeling. Examples from

well-established parallel programming systems (HPF and MPI) will be included. After the basic material is covered, we will examine two new programming systems for parallel machines, OpenMP and PETSc.

7.5.10 An Introduction to the Fortran 90

This course is aimed at introducing engineers and scientists familiar with Fortran 77 to the new features and capabilities available in Fortran 90. These new features include free-form source code, the CASE control structure, the ability to create new data types, modules (similar to C++ courses), array processing shortcuts, dynamic memory allocation, pointers, improved I/O handling, and a host of new intrinsic functions. Source code compatibility between Fortran 77 and Fortran 90 will also be discussed.

7.5.11 Scalable OpenMP Programming on Origin2000

This is an advanced course. Topics to be covered are as follows:

- Overview of OpenMP programming model.
- Review of execution model.
- Moving beyond incremental parallelization mode.
- Domain decomposition.
- Comparisons with message passing.
- Performance optimization on Origin 2000.
- Preview of OpenMP C/C++ specification.
- Introduction to MSC/PATRAN Modeling for Design Analysis

This is an introductory course for the new and/or infrequent MSC/PATRAN user. Students will master the basic skills required to use MSC/PATRAN in a typical MCAE application. The course emphasizes practical skills development through comprehensive, hands-on laboratory sessions. Students will learn to build analysis models using MSC/PATRAN, by defining material properties, creating boundary conditions, and submitting their problems for analysis and post-processing the results using a variety of graphical formats. Specific topics such as CAD integration, geometry editing, meshing, grouping, and customization will be covered. Users of all FEA codes are encouraged to attend since MSC/PATRAN supports all the popular FEA codes such as MSC/NASTRAN, MSC/DYTRAN, HKS/ABAQUS, ANSYS, LS-DYNA and many more.

7.5.12 TANGO for Remote Consulting

NPAC's TANGO is a Web collaboratory. The system extends capabilities of Web browsers towards a fully interactive, multimedia, collaborative environment. TANGO is also a framework for building collaboratory systems. In this tutorial we will instruct how to use TANGO and will cover applications of TANGO for remote consulting, including all critical software development phases: coding; compiling; testing and debugging; and result analysis.

7.5.13 Parallel Debugging and Performance Analysis Tools: TotalView and Vampir

This course introduces parallel application developers to parallel debugging and performance analysis tools available on CEWES MSRC platforms, and provides more in-depth coverage of the TotalView debugger and Vampir performance analysis tool. The course will cover the basics of using the tools as well as provide pointers to further information. A lab session will include practice on using the tools on some example programs. Debuggers to be covered include: Dolphin (which is now Etnus, Inc.) TotalView 3.8 for the SGI/CRAY Origin2000 and IBM SP; CRAY TotalView for the CRAY T3E; SGI dbx for the Origin2000; and pdbx for the IBM SP. Dolphin TotalView has a graphical interface while dbx and pdbx provide command-line debugging interfaces. The Cray version of TotalView for the CRAY T3E has both graphical and command-line interfaces. An overview will be given of the various performance analysis tools available on CEWES MSRC platforms, but the performance analysis portion of the course will focus in detail on the Vampir tool, which has been recently acquired and is now available on CEWES MSRC machines.

7.5.14 Techniques in Code Parallelization

The techniques needed to parallelize an algorithm and code are described. These include: discretization methods, domain decomposition, linear and nonlinear solver issues, mesh partitioning, load balancing, pre processing, and post processing. Examples of parallelization efforts carried out at the University of Texas will be given. Participants will also have a chance to bring their "dusty deck" codes for discussion on how best to migrate them to parallel platforms.

7.5.15 Parallel Programming on the SGI/CRAY Origin2000 using OpenMP

This "how-to" workshop is designed to train the participants in the techniques and tools required to perform parallel programming using OpenMP directives on the Origin2000(O2K). After a discussion of the MIPS R10000 processor, the O2K architecture, and an introduction to the IRIX operating system creation and

scheduling of parallel threads, the OpenMP directives will be discussed in detail along with examples of their use. The course will conclude with the equally important topic of how to distribute the data used by parallelized OpenMP regions among the local memories on the O2K.

7.5.16 Computational Monitoring Using CUMULVS

Computational monitoring lets you visualize simulation output while your computation executes. This can be useful for users with codes that produce very large output files, or when you want to stop a run that is not progressing satisfactorily. This "how-to" workshop will educate participants in the techniques and procedures required to perform interactive computation using currently available tools. The workshop will include the following:

- An overview and discussion of available tools, commercial or freeware.
- An introduction to CUMULVS from Oak Ridge National Lab.
- Detailed steps for how to instrument your code to use CUMULVS.
- Discussion of possibilities for computational monitoring for participants' codes.

7.5.17 Interactive Structured Time-varying Visualizer (ISTV)

This tutorial gives an introduction to the Interactive Structured Time-varying Visualizer (ISTV), an OpenGL-based scientific visualization package available on IRIX and Solaris. ISTV is an interactive visualization system that visualizes time-varying multi-block (or multi-grid) simulations on time-varying grids. ISTV's genesis was in the need for a toolkit to visualize data from high-resolution ocean models. By exploiting modularity and plug-ins, the scientist has the ability to tailor the ISTV visualization system to the needs of a particular discipline or problem without having to write a completely new system.

7.5.18 WebFlow: Web Interfaces for Computational Modules

In this course we will present the WebFlow system developed at Northeast Parallel Architectures Center (NPAC) at Syracuse University. This system addresses the needs for high level programming environments and tools to support distance computing on heterogeneous, distributed platforms. During the course we will describe and demonstrate the WebFlow system. This will include background information on CORBA and developing CORBA objects in Java. We will present

the architecture of WebFlow, discuss its security model, and methods of providing a seamless access to remote resources. The course will focus on applying WebFlow to the users' applications. We will explain how to customize the WebFlow front-end to the needs of a particular application, and how to invoke and control the users' computational modules.

This page intentionally left blank

8. SUPPORT of CEWES MSRC USERS

Since the great majority of users of the CEWES MSRC are off-site, the CEWES MSRC PET effort places emphasis on outreach to remote users, as well as to users located on-site at CEWES. Table 3 lists the contacts made with CEWES MSRC users by the CEWES MSRC PET team during Year 3, and Table 2 lists all travel by the CEWES MSRC PET team in connection with the Year 3 effort. A major component of outreach to CEWES MSRC users is the training courses (described in Section 7) conducted by the CEWES MSRC PET team, some are conducted at remote user sites and some are Web-based. The CEWES MSRC PET Web site, accessible from the CEWES MSRC Web site, is also a major medium for outreach to CEWES MSRC users, and all material from the training courses is posted on the PET Web site. A CD-ROM of training material has also been prepared.

Specific support activities conducted in Year 3 are described in this section, which is organized by individual components of the CEWES MSRC PET effort.

8.1 CFD: Computational Fluid Dynamics CTA (ERC - Mississippi State)

Through core support, the CFD team was able to provide training and user support and outreach via participation in Parallel Programming Workshops for Fortran Programmers (Bring Your Own Code: BYOC), MPI tutorials, and direct CEWES MSRC user contacts.

Interactions with CEWES MSRC users have been initiated by a variety of means. Telephone, E-mail, and personal visits have all resulted in opportunities for user support and more specific collaborative efforts. Face-to-face visits have resulted from training participation such as the Parallel Programming Workshop for Fortran Programmers (BYOC) where users are introduced to parallel programming within the context of their own code. This is a particularly effective opportunity for user outreach and training, since it gives the On-site CTA Lead (Bova) an opportunity to meet and interact with users on an individual basis and learn about their work within a semi-formal classroom environment. Some of the more significant outreach interactions are described below.

In collaboration with Henry Gabb, Computational Migration Group (CMG) at CEWES MSRC, assistance was provided to J. C. T. Wang of the Aerospace Corporation by analyzing the message flow in a section of his PVM code and with general support resulting in a successful code port to the IBM SP system. David Medina of AF Phillips Lab implemented a graph-based reordering strategy within the MAGI solver resulting from PET consultation. The objective was to improve

cache performance and interprocessor data locality. Results report about a 30% execution time reduction for two, four, and sixteen processors compared to execution without reordering. Interaction with Fernando Grinstein of NRL has continued in the third contract year. Collaboration via phone, E-mail and personal visits occurred in order to provide user assistance in development of a parallel version of NSTURB3D capable of efficient execution on all CEWES MSRC computing platforms.

A dual-level parallel algorithm using both MPI and OpenMP was designed and implemented into the CGWAVE solver supporting Zeki Demirbilek of CEWES. This resulted in dramatic reduction in turnaround time. Turnaround time for the demonstration case was reduced from 2.1 days to 12 minutes using 256 SGI O2K processors. This project also involved extensive collaboration with the SPP Tools team, and Tennessee and served as a test bed for their MPI_Connect Tool.

Collaboration with Bob Robins of NW Research Associates occurred as a result of the BYOC workshop, via follow-up email, and phone contact. His code has been analyzed for inherent parallelism, and continued collaboration to produce a parallel version of his solver has been offered.

Specific support was provided to two CHSSI development teams:

CFD-2 (COBALT Unstructured Gridding - Bill Strang, NRL): Coordination with Hank Kuehn resulted in a special queue priority for the COBALT development team to assist in timely debugging of their solver. This helped identify an implementation problem that only manifested itself for applications using more than forty processors.

CFD-4 (OVERSET Chimera Gridding - Robert Meakin, Army Aeroflightdynamics Directorate at NASA Ames Research Center): The CFD team worked to secure FY99 allocation on CEWES MSRC hardware for the OVERFLOW development team.

8.2 CSM: Computational Structural Mechanics CTA (TICAM - Texas, with ERC - Mississippi State)

The first step in outreach to CSM users was the short course on Finite Element Analysis of Nonlinear Problems at the DoD HPCMP Users Group Meeting at Rice in June 1998. We also lectured on adaptive techniques and multi-scale modeling at the Workshop on Recent Advances in Computational Structural Mechanics and High Performance Computing held at CEWES in November 1998 and organized a

workshop on Adaptive Techniques, Error Indicators and Applications held at Texas in March 1999.

Rick Weed, the CSM On-site Lead, has been instrumental in coordinating our interactions with the applications analysts at CEWES and elsewhere. For example, during the Workshop in November at CEWES, we met with on-site engineering analysts involved in application studies using CTH and EPIC. Follow up was made at the February PET Annual Review by Carey and Littlefield with the EPIC analysts to discuss our recent adaptive grid capability. As a result of this meeting, we mapped a strategy for collaborating with the users and for testing their nonlinear material models in our adaptive EPIC code. We also developed a goal for a parallel roadmap task and CEWES MSRC code migration plan to be undertaken in Year 4 or the following year.

David Littlefield has been in regular close contact with the major CSM users at ARL (K. Kimsey, D. Scheffler, D. Kleponis). We have had several discussions with Raju Namburu, CSM CTA Lead, and recently discussed tech transfer to transition the adaptive CTH code version. This transfer is being coordinated with Gene Hertel and the Sandia group.

8.3 CWO: Climate/Weather/Ocean Modeling and Simulation CTA (Ohio State)

Sadayappan and Welsh of Ohio State had three major coordination meetings with Bob Jensen of CEWES during PET Year 3. These meetings were to plan ongoing efforts on the parallelization and migration of the WAM wind-wave model, and the coupling of WAM with the CH3D marine circulation model. SGI on-site representative Carol Beaty at CEWES MSRC was present at the first and second meetings, and government CWO monitor Alex Carillo at CEWES MSRC attended the second and third meetings. There were numerous E-mail and telephone contacts with Bob Jensen throughout the year, and Welsh made four additional one-week trips to CEWES MSRC to provide CWO core support.

At the May 1998 WAM coordination meeting, a major topic was the disagreement of predictions of the pre-existing (MPI-based) parallel WAM code with those of the original sequential WAM code. Subsequent debugging traced the problems in MPI WAM to shallow water, current-related propagation effects and inter-grid communication in nested grid runs. The coding errors responsible for the problems were not found, however, and it was agreed shortly after the August 1998 coordination meeting to replace MPI WAM with an OpenMP version of WAM. The OSU team then deployed OpenMP WAM in the coupled CH3D/WAM system.

Apparent errors in the WAM treatment of current-induced wave refraction were also discussed at the May 1998 WAM coordination meeting. Welsh subsequently examined the WAM propagation scheme and found a sign error repeated several times in the main propagation subroutine. A corrected version of the subroutine was delivered to Bob Jensen.

In May 1998, Welsh also met with Bob Jensen, Don Resio, and Linwood Vincent of CEWES to review the coupling physics being implemented in the CH3D/WAM system. This meeting resulted in a modification of the WAM bottom friction algorithm.

At the October 1998 WAM coordination meeting, the major issue was the unexpected termination of OpenMP WAM simulations on the SGI Origin2000. Follow-up work with Carol Beaty and Computational Migration Group staff at CEWES MSRC (Henry Gabb and Trey White) showed that explicit stack size specification was necessary, and that aggressive optimization during code compilation caused small errors in the WAM results. Welsh also found that if the WAM grid is trivially split into one block (the computational grid is divided in to a user-specified number of blocks to save memory), the simulation will terminate unexpectedly.

In May 1998, Sadayappan and Zhang of Ohio State traveled to Mississippi State to meet with Billy Johnson of CEWES. The purpose of the trip was to discuss the physics required for the coupling of CH3D and WAM at the atmospheric boundary layer, and the coupling of CH3D-SED and WAM at the bottom boundary layer. The parallelization of CH3D-SED was also planned with Puri Bangalore of MSU. CH3D-SED was subsequently parallelized by MSU staff, and the parallelization was verified by OSU staff.

In March 1999, CWO On-site Lead Steve Wornom met with Lori Hadley and Bob Jensen of CEWES and SPP Tools On-site Lead Clay Breshears, and Henry Gabb and Ben Willhoite of the Computational Migration Group, to discuss the parallelization of the SWAN wind-wave model. This resulted in a joint CWO/CMG/SPP Tools effort to migrate the code to the CEWES MSRC parallel platforms.

8.4 EQM: Environmental Quality Modeling and Simulation CTA (TICAM - Texas)

The EQM team working with Mark Noel of CEWES had verified version 1.0 of parallel CE-QUAL-ICM in December of 1997, and in March of 1998, the first 10-year Chesapeake Bay calibration run had been completed for the EPA.

Starting in April 1998, we interacted mainly with Mark Noel to add features to the parallel code needed to run the EPA scenarios. We also trained him to write routines for post-processing parallel runs. From March through September 1998, Noel was able to run 53 10-year calibration runs, and 53 actual runs for the EPA Chesapeake Bay project, using a total of 24,663 CPU hours. The EQM team gave a joint presentation with Mark Noel of CEWES at the DoD HPCMP Users Group Meeting in June 1998.

In November 1998, Carl Cerco of CEWES asked us to help improve the scalability of CE-QUAL-ICM for future planned large-scale work. We analyzed the parallel code using a 10-year Chesapeake Bay run as a benchmark, and improved parallel CE-QUAL-ICM in several respects. These improvements required interaction with Mark Dortch, Carl Cerco, Mark Noel, and Barry Bunch of CEWES. We improved the I/O performance and developed techniques, which allowed the code to run on more CPUs (up to 110) with good parallel performance. The new code was verified by the end of February 1999.

Discussions with Mark Dortch, Carl Cerco, Barry Bunch, and Mark Noel of CEWES led us to improve the grid decomposition algorithms crucial to our method of parallelization. We investigated the use of the grid partition package METIS 4.0 and built an interface to this package, which greatly improved the scalability of CE-QUAL-ICM. Mark Dortch asked the EQM team to help transfer the parallel computing technology to the toxic version of the code. We trained Terry Gerald and Ross Hall of CEWES in the basic techniques, and on their own they were able to code a parallel version of CE-QUAL-ICM/TOXI. Similarly, Fred Tracy of CEWES was able to parallelize FEMWATER on his own after attending our Workshop on Parallel Technologies held at CEWES MSRC in January of 1998 by patterning his approach after ours. Tracy reported on his results at the DoD HPCMP Users Group Meeting at Rice in June 1998.

8.5 FMC: Forces Modeling and Simulation/C4I CTA (NPAC - Syracuse)

Currently, our main DoD FMS user group that provides the application focus and testbed for the WebHLA framework is the Night Vision Lab at Ft. Belvoir (Army) which develops CMS (Comprehensive Mine Simulator) as part of their R&D in the area of counter-mine engineering. Our support for CMS includes:

Building Parallel CMS module by porting sequential CMS to the Origin 2000 (and later to a commodity cluster).

Integrating Parallel CMS module with other WebHLA federates (JDIS, PDUDB, SimVis).

Planning future joint work with Ft. Belvoir. This includes development of joint proposals such as a currently pending CHSSI proposal on WebHLA for Metacomputing CMS.

We are also interacting closely with and providing PET support for current FMS CHSSI projects:

FMS-3 (Efficient PDESS for Analysis - Bill Smith, NRL): We are building Web-based interactive training for the SPEEDES simulation kernel.

FMS-4 (HPC Frameworks for Wargaming and Training Simulations - Larry Peterson, NOSC): We are acting as external technical reviewer and recently developed a joint CHSSI proposal with SPAWAR for a follow-on project on using SPEEDES, Parallel IMPORT and WebHLA to build Intelligent Agent support for FMS.

FMS-5 (HPC High Level Architecture Runtime Infrastructure - Jeff Wallace, Space and Naval Warfare Systems Center): We expect to directly participate and were asked to provide our Object Web RTI as a test implementation of the RTI 1.3 standard, to be certified by DMSO and used by FMS-5 as a fully compliant reference prototype.

8.6 C/C: Collaboration and Communications (NPAC - Syracuse)

Since our primary C/C effort in Year 3 focused on the TANGO Interactive electronic collaboration system for use in education, training, and small-group collaboration, our outreach efforts focused on enlarging the base of knowledgeable and experienced users of the system as a base to help support broader deployment of the tools. This work was conducted with on-site Training and C/C (or equivalent) support personnel at the four MSRCs, as well as with staff at the Naval Research Lab in DC. Our collaborators at the Ohio Supercomputer Center (a PET partner) gained experience not only in operation and support of TANGO from the course recipients' point-of-view, but also as instructors. All four MSRCs, as well as OSC, now have TANGO server installations, and along with NRL have substantial experience with the client side of the system. This group of experienced users will form a core of support that will facilitate wider use of TANGO for both training and other collaborative applications in the coming years.

8.7 SPP Tools: Scalable Parallel Programming Tools (CRPC - Rice, Tennessee)

Our SPP Tools On-site Lead, Clay Breshears of Rice, had major impact during Year 3 working with users at CEWES MSRC and other DoD sites. Rice hosted the DoD HPCMP Users Group Meeting held in June 1998, and we gave five

tutorials. Over 350 attended the meeting. This required a large effort from the SPP Tools Lead at Rice University and the Rice support staff. SPP Tools Senior Academic Leader Prof. Ken Kennedy (Rice) gave the keynote address at the meeting. Additionally, Prof. Richard Smalley (Rice), 1996 Chemistry Nobel Laureate, was a featured speaker during the conference.

Many users were provided with critical help on upgrading their application codes or other programming-related issues. Support of CEWES MSRC users during Year 3 by the SPP Tools team included the following specific assists:

Marvin Moulton (NASA Ames Research Center): Contact made though Steve Bova, On-site CFD Lead, for information about the HELIX code.

David Medina (AF Phillips Lab): Various E-mail exchanges and various telephone contacts for information about the MAGI code. MAGI code is being studied at Rice as a testbed of compiler optimization studies.

Fred Tracy (CEWES): On possible collaboration on optimization of FEMWATER.

Ann Sherlock and Jane Smith (CEWES): On possible collaboration of parallelization of STWAVE and tutoring program at Rice.

Zeki Demirbilek (CEWES): Clay Breshears implemented MPI_Connect version of CGWAVE code. This effort was in collaboration with other members of CEWES MSRC PET, the Computational Migration Group at CEWES MSRC, the CEWES MSRC Computational Science and Engineering group, and the University of Tennessee. The code won the Most Effective Engineering Methodology Award from the SC98HPC Challenge competition.

Bob Robins (Northwest Research Associates, Inc.): Found potential Fast Poisson Solver libraries during BYOC workshop held at CEWES MSRC.

Chuck Koelbel, Gina Goff, and Ehtesham Hayder offered tutorials at CEWES MSRC and at NRL and discussed with the participants their codes and possible ways of parallelization.

Clay Breshears assisted the CEWES MSRC Computational Science and Engineering (CSE) group members with the use of the Vampir performance analysis tool and the TotalView debugger. Also, he was able to help members of the RF Weapons Challenge Project (Kirtland AFB) with these tools.

Tennessee has worked with CEWES MSRC user and CEN-1 (Scale Algorithms for Dynamic Nonlinear Simulations) CHSSI code developer David Rhodes of the Army CECOM Research Development and Engineering Center to use the Vampir performance analysis tool to analyze and improve the performance of the Harmonic Balance Simulation code. Rhodes reports the following:

"The Vampir toolset provided just what I was looking for in tuning my parallel application. This application contains tasks that range from small to large granulity. Vampir allowed me to view dynamic program execution with a very low level of intrusion. After making some significant algorithmic changes — e.g. changing from a dynamic to static scheduling approach. I was able to achieve much better levels of scalability and parallel efficiency. The data needed to determine existing problem areas would have been much harder to gather without Vampir."

Tennessee has worked with two members of the RF Weapons Challenge Project team, Gerald Sasser and Shari Collela, of AF Phillips Lab in their use of Vampir. Vampir was used by Sasser to find and fix a bottleneck in the ICEPIC code and to significantly improve the communication performance of that code. Collela has been unsuccessful so far in using Vampir on the Mach3 code because the code is very large and produces huge and unwieldy trace files. Tennessee plans to use the Mach3 code as a test case for new dynamic instrumentation techniques that can be used to dynamically turn Vampir tracing on and off, and thus reduce the size of the tracefiles while still collecting trace data for "interesting" parts of program execution.

Graham Fagg of Tennessee worked with the CEWES MSRC team to use Tennessee's MPI_Connect system, along with OpenMP and MPI, to achieve multiple levels of parallelism in the CGWAVE harbor response simulation code of CEWES, which reduced the runtime for this code from months to days. The team won the Most Effective Engineering Methodology award for their SC98 HPC Challenge entry.

Tennessee has tested the installed versions of the tools and has worked with CEWES MSRC systems staff to ensure that the tools are working correctly in the programming environments used by CEWES MSRC users, including the PBS queuing system. Tennessee has also reported to the tool developers any bugs discovered and followed up on getting them fixed. An E-mail message about the SPP Tools repository was sent to CEWES MSRC users, and an article about it has been written for the CEWES MSRC Journal. The repository and the tools have already had an impact on the Computational Migration Group (CMG) at CEWES MSRC, which has started using some of the tools such as TotalView on a daily

basis to do their jobs more effectively. The CMG is encouraging other CEWES MSRC users to do likewise.

8.8 SV: Scientific Visualization (NCSA - Illinois, with ERC - Mississippi State)

During Year 3, the PET visualization team worked with CEWES MSRC users, the PET on-site staff for each CTA, and the CEWES MSRC visualization staff.

Early in the year, we surveyed several CEWES MSRC users to discuss their data management strategies. This led to the summary report in which we recommended that HDF, a data management package in use by NASA EOSDIS and DOE's ASCI project, be introduced to the CEWES MSRC. In July, we arranged for HDF project lead, Dr. Mike Folk of NCSA, to visit the CEWES MSRC and present an overview of HDF.

We also worked with a variety of CEWES MSRC users to assist in visualization production. We worked with Andrew Wissink (MCAT - NASA Ames Research Center) to produce a visualization of his store separation problem. Still imagery and time-series animations were produced for Robert Jensen of CEWES. Additional visualization production was undertaken with Carl Cerco's data (CEWES). This includes a movie sequence that can take advantage of the very-wide screen (the Panoram) installed at the CEWES MSRC.

The PET Vis team has had a long-term relationship with Bob Jensen of CEWES, particularly as it relates to customizing visualization tools to support his wave modeling work. We also work with Raju Namburu's team (CEWES) on novel application of wavelet techniques to build structure-significant representations of his data. This is particularly important as Namburu's datasets are very large.

In another long-term collaboration, the PET Visualization team has ongoing communication with Carl Cerco, Mark Dortch, and Mark Noel of CEWES, in relation to their Chesapeake Bay project and visual analysis of the output of the CEWES CE-QUAL-IQM code. This is a continuation of the relationship that was begun in Year 1. This year, we have worked with them on defining their requirements for desktop visualization support, prototyping solutions for those needs, and iterating on the design process to refine their specifications. We have provided them a production-quality version of a tool that they are currently using to view data from their 10- and 20-year productions run of the Chesapeake Bay model. This tool also supports a limited form of collaboration that they are using to share their results with their project monitor at the Environmental Protection Agency.

The CEWES PET SciVis team has had a variety of contacts with the PET CTA on-site staff, including Steve Bova (CFD) and Rick Weed (CSM), to consult on how to best assist their users in the areas of computational monitoring and visualization. Also, we have worked with our PET academic counterparts, Professors Mary Wheeler (EQM, Texas), Keith Bedford (CWO, Ohio State), and Geoffrey Fox (FMS and C/C, Syracuse).

In Year 3, we also had numerous contacts with CEWES MSRC visualization personnel, including Dr. Michael Stephens, Dr. Richard Strelitz, Dr. Kent Eschenberg, Richard Walters, and John West. We have advised on new software packages and techniques for visualization and virtual environments. We also have continuing contact with Milti Leonard, visualization staff at Jackson State University, consulting on visualization software and mentoring her in her own skill development.

MSU's major SV interaction has been with CSM scientist Raju Namburu of CEWES. He has guided the project and has influenced the quality deliverables to a great extent. In addition, he also explored the use of several algorithms including volume rendering for his datasets and has spurred the development of tools to aid the main project.

Finally, we conducted both informal and formal training sessions. A half-day "Introduction to HDF" was presented at both the CEWES MSRC and at Jackson State. A day-long class introduced the various packages that exist for supporting computational monitoring, such as CUMULVS, DICE, and pV3. In Year 4, we intend to convert the material developed for this class to an on-line format, so the information will be available at any time for continuing impact. Another training day discussed the use of the visualization tool ISTV. These courses have led to follow-up and continuing contact with CEWES MSRC users.

8.9 University of Southern California

The USC team met with Dr. Rama Valisetty of CEWES MSRC to discuss the computation and communication structure of key applications in Computational Structural Mechanics (CSM). This interaction helped us focus our benchmarking and modeling efforts to accommodate the problems that real end-users face in parallelizing their code.

The USC team interacted with a DoD end-user through Valisetty. An unoptimized CFD application was given to USC. USC employed the benchmark results and the IMH model to initially analyze the computation and communication requirements of the original algorithm. A flow diagram was then created and the major

bottleneck sections of the code were identified. Using the IMH model, the USC team analyzed the performance of various data reorganization techniques, communication latency hiding techniques, and computation scheduling choices. This allowed USC to optimize the algorithm to minimize the communication overhead of parallelization while distributing the workload evenly among the processors. The optimized algorithm developed by USC was scalable and portable. Using 30 processing nodes, the performance was improved by approximately 5 fold over the original algorithm.

8.10 Clark Atlanta University

There was continual interaction with Raju Namburu of CEWES from the ViSiDeL group. Gary Jones was stationed at CEWES MSRC in July 1998 and had successful work interaction with Namburu. Olatidoye visited CEWES MSRC for a technical project review with Namburu in July 1998. There was continual remote telephone interaction between Olatidoye and Jones with Namburu on computer code development for the Damage Structure Test bed at the ViSiDeL. This interaction led to a unique method of rendering large structural (and similar) datasets without creating a memory burden to the corresponding visualization packages. The Integrated CAD-FEM Method involves not only integrating the CAD modeling aspect of CSM applications with the finite element mesh (FEM) generation process, but also re-mapping the FEM results back to the original CAD model.

This page intentionally left blank

9. HBCU/MI ENHANCEMENT PROGRAM

For Year 3, the Historically Black Colleges and Universities/Minority Institutions (HBCU/MI) team for the DoD HPCMP consisted of Jackson State University (JSU), Central State University (CSU), and Clark Atlanta University (CAU). JSU, located in Jackson, MS, is the lead HBCU/MI at the CEWES MSRC. CSU, located in Wilberforce, Ohio, is the lead for the ASC MSRC, and Clark Atlanta University (CAU), located in Atlanta, Georgia, is the lead at the ARL MSRC. While each university plays the major role at its home MSRC, with respect to the HBCU/MI program, each institution is also committed to making technical contributions to the PET effort, and to the overall DoD HPC Modernization Program effort.

Prof.Willie Brown of Jackson State is the overall HBCU/MI Senior Academic Leader for CEWES MSRC PET.

This section describes how these institutions participated in PET initiatives at the CEWES MSRC during the third year of the program, and how the institutions were enhanced by their involvement. Training courses and seminars conducted by the CEWES MSRC PET team at HBCU/MIs are listed in Table 8.

As the lead university at the CEWES MSRC, JSU is charged with developing and implementing strategies that allow a two-way exchange between the DoD and HBCU/MI communities. Minorities are tremendously underrepresented in the Computational Technology Areas (CTAs) and other HPC efforts within the DoD, and the existing pool of talent available to address current and future DoD challenges, using HPC technologies, is limited and decreasing. The PET program provides the DoD with an opportunity to identify and develop new sources of scientific, high-tech, and management personnel. In the opposite direction, PET affords faculty, staff, and students, at HBCU/MIs, an opportunity to acquire scientific and HPC related skills and expertise through interaction with DoD scientists and researchers. JSU's mission is to maximize mutual benefit for both sides by helping to create and maintain pathways between the CEWES MSRC and the HBCU/MI team. However, adequate access to HPC facilities, and other information technology resources, is critical to HBCU/MI participation in this endeavor.

9.1 PET Team at Jackson State

The JSU support team for the CEWES MSRC consists of five members. Prof. Willie Brown is the overall HBCU/MI Academic Leader for CEWES MSRC PET, as well as Academic Leader for Jackson State. At JSU, Brown is responsible for

overall management of PET activities at JSU, including core support and focused efforts. Jeton McClinton serves as administrative assistant for the project. She is responsible for bookkeeping, travel arrangements, and clerical support of all other JSU personnel. Milti Leonard and Edgar Powell provide scientific visualization support for CEWES MSRC personnel and scientific visualization training for JSU students, faculty, and staff. Leonard and Powell work closely with PET partner NCSA at the University of Illinois. Michael Robinson is the JSU Network Training Lead and is responsible for technical support of the JSU Distance Education effort. This includes hardware/software set-up and maintenance, as well as classroom teaching assistance.

JSU's role in CEWES MSRC PET is two-fold. First, JSU is the lead, Historically Black College/University (HBCU). In this role, JSU's primary mission is to identify, and make available to the CEWES MSRC, high performance computing (HPC) capabilities and expertise at targeted HBCUs and other Minority-Serving Institutions (MIs). The co-mission is to identify, and make available to those targeted HBCU/MIs, opportunities for HPC training and capability development/enhancement. The second JSU PET role is strictly technical. Two focused efforts are in operation: Distance Education, and Scientific Visualization.

9.2 PET Team at Clark Atlanta

The CAU CSM effort is lead by Prof. Olu Olatidoye, the Principal Investigator on the "Damage Assesment and Residual Evaluation of Structures". Members of the team are Gary Jones, a Research Engineer/graduate student working on code enhancement. Dr.Prakash Sarathy, a co-investigator that worked on the project during the Summer of 1998. Leon Milligan (undergraduate student), Eddie Mason (undergraduate student) and Clauzel McIntyre (graduate student) are research students that contributed to the project. Ravena Baskerville-Lottie, the Program Manager for the ViSiDeL coordinates the reports and Kweli Walker, the Office Manager, handles the budget.

9.3 Jackson State HPC Summer Institute

In support of its HBCU/MI missions, JSU continued communication and collaboration with other PET HBCU/MIs (Central State University, Clark Atlanta University, Dillard University, and Morgan State University). In addition, JSU hosted the second annual Introductory High Performance Computing Summer Institute, June 8 - 19, 1998. At the institute, presenters from seven CEWES MSRC PET team universities introduced twenty students from six HBCUs to HPC in general, and to the computational technology areas (CTAs) supported at the CEWES MSRC. PET universities represented were Illinois (NCSA), Mississippi

State (ERC), Ohio State (OSU), Rice (CRPC), Syracuse (NPAC), Texas (TICAM), and JSU. Students came from Alcorn State, Dillard, Florida A&M, Mississippi Valley State, Tougaloo College, and JSU.

9.4 Jackson State Distance Learning

During Year 3, JSU and PET partner Syracuse teamed up to present four distance education courses over the Web. Syracuse delivered one undergraduate course (Web Programming) and two graduate courses (Computational Science for Simulation Applications, Advanced Web Programming) to JSU, while JSU delivered one undergraduate course (Web Programming) to Morgan State University. Syracuse also delivered the Advanced Web Programming course to Mississippi State and Clark Atlanta. All offerings were full semester, for-credit courses delivered over the Web using the TANGO collaborative software environment. The JSU-Syracuse communications link was implemented on the Defense Research and Engineering Network (DREN).

9.5 Jackson State PET Technical Support

JSU worked with PET partner NCSA to provide scientific visualization training and support to CEWES MSRC users. Specifically, JSU's efforts focused on remote scientific visualization, i.e. enabling technologies that allow users in geographically distributed locations to access visualizations generated at remote sites.

9.6 Clark Atlanta PET Technical Support

In the Clark Atlanta (CAU) Year 3 effort, a comprehensive understanding of the input format for Dyna3d has been obtained through various studies. A general translator has been written which reads CAD mesh data and converts it into Dyna3D nodal and element data. The translator accepts CAD models that contain four node shell elements, eight node thick shell elements, and eight node brick elements. Material properties and load curve specifications for the translator are still under development.

In addition, the overall framework for visualizing and assessing the damage of a structure has been defined by the following three levels of visualization:

The local material stresses will be displayed for the entire structure.

All failures of specific members will be shown based on accepted structural analysis limit states.

An indication of the residual capacity of the structure will be displayed for various sections of the building.

Each level of visualization will be rendered in the DOISE virtual environment.

Furthermore, a parallel post-processing code was modified to translate Dyna3D plot files into a format which can be read by DOISE. The code outputs geometric data as well as stress, strain, and moment data for the specified time steps of a given simulation.

As part of the CEWES MSRC DoD user community, there was strong collaboration and interaction with Raju Namburu at CEWES. Significant enhancement of model prediction capability for use in damage control has occurred. This will also enhance the prediction of explosive effects, which has an impact on the Challenge Problem on Damage Structures.

10. CEWES MSRC/PET TECHNICAL REPORTS

98-43 G. C. Fox, W. Furmanski, S. Nair and Z. Odcikin Ozdemir, "Microsoft DirectPlay meets DMSO RTI for Virtual Prototyping in HPC T&E Environments", CEWES MSRC/PET TR/98-43, Vicksburg MS, 1998.

Abstract:

In our Pragmatic Object Web approach to distributed object technologies, we integrate complementary aspects of CORBA, Java, COM, and WOM. Here, we focus on Microsoft COM and we analyze synergies between DirectX / DirectPlay multi-player multimedia gaming technologies and the DoD Modeling and Simulation technologies such as HLA/RTI. We discuss the integration of both layers via the COM/CORBA bridge using our JWORB (Java Web Object Broker) middleware. We outline an early draft of a Web/Commodity based High Performance Virtual Prototyping Environment for Testing, Evaluation and Simulation Based Acquisition that will integrate commodity software (DirectX) and hardware (NT clusters) with the legacy simulation backends.

98-44 G. C. Fox, W. Furmanski and H. T. Ozdemir, "Object WEB (Java/CORBA) based RTI to support Metacomputing M&S", CEWES MSRC/PET TR/98-44, Vicksburg MS, 1998.

Abstract:

We present our Pragmatic Object Web based approach to High Performance Modeling and Simulation and describe the associated middleware software recently prototyped at NPAC: JWORB (Java Web Object Request Broker) integrates HTTP and IIOP protocols, and Object Web RTI implements DMSO RTI 1.3 on top of the JWORB-based CORBA / Java software bus. We explain how JWORB and OW RTI are used to build WebHLA — an interactive FMS training environment and outline our plan towards WebHLA-based Virtual Prototyping Environments for Testing, Evaluation, and Simulation Based Acquisition.

98-45 Marek Podgorny and Geoffrey C. Fox, "Real Time Training and Integration of Simulation and Planning using the TangoInteractive Collaborative System", CEWES MSRC/PET TR/98-45, Vicksburg MS, 1998.

Abstract:

We describe TangoInteractive, a Web-based collaborative system which has shown promise in several prototype activities and can be deployed in a large-scale fashion over the next two years. We present it in terms of a general taxonomy of collaborative or groupware systems represented by other commercial and research activities including Lotus Notes, NetMeeting from Microsoft, and Habanero from NCSA. We then describe two applications: 1) command and control and 2) distance learning where we have implemented successful prototype and which represent areas similar to those of interest to the Test and Evaluation Community. We give lessons from this initial work.

98-46 Geoffrey C. Fox, W. Furmanski and T. Pulikal, "Evaluating New Transparent Persistence Commodity Models: JDBC, CORBA PSS, OLEDB and W3C WOM for HPC T&E Databases", CEWES MSRC/PET TR/98-46, Vicksburg MS, 1998.

Abstract:

We analyze the standard candidates for the universal (storage medium- and vendor-independent) persistency frameworks as proposed by the leading alternative technologies for distributed objects: Java, CORBA, COM, and WOM. We point out that the consensus in this field is yet to be reached and present our Pragmatic Object Web approach to coordinate and integrate complementary technologies. We illustrate it on a few practical examples of Web linked collaboratory database environments constructed recently for various communities and application domains such as telemedicine, distance education, interactive FMS training, and data mining of T&E data from the Virtual Proving Ground. Finally, we summarize lessons learned and outline our recommendations for the HPC T&E database approach.

98-47 Remek Trazaska, Scott Klasky, Tomasz Major, Marek Podgorny, Geoffrey C. Fox and David E. Bernholdt, "TANGO Interactive for Remote Consulting and Group Software Development", CEWES MSRC/PET TR/98-47, Vicksburg MS, 1998.

Abstract:

NPAC's TANGO has proven to be an excellent tool in distance education and corporate training situations. The environment we developed in NPAC for this project extends the areas of TANGO applications to distance consulting. The set of tools we prepared allows geographically dispersed programmers and application designers to work together on complex short-term (consulting) or longer-term (software development) efforts as if they were working at the same location.

98-48 Kent Eschenburg and Mike McCraney, "Virtual Prototype Radio Frequency Weapon Project Visualization: A Case Study", CEWES MSRC/PET TR/98-48, Vicksburg MS, 1998.

Abstract:

At the 1997 DoD HPC User Group meeting, the Virtual Prototype Radio Frequency Weapon Project was described as "...an ambitious effort to use newly-developed plasma, particle beam, and electromagnetic codes to design useful high power radio frequency (RF) weapons components via parallel computation." (Ref. 1) This paper describes the methods used by the Scientific Visualization Center at the CEWES MSRC to work with these remote users to visualize the ICEPIC portion of the simulation. Some useful methods developed for this effort include: a preprocessor that resamples the electron field to produce a compact file for viewing; a combination of custom and commercial code for the visualization; and a dual visualization approach where components are developed at CEWES MSRC and then sent to the customer for reuse on their workstation.

98-49 S. W. Bova, C. P. Breshears, H. A. Gabb, "Status Report on Parallelization of MAGI", CEWES MSRC/PET TR/98-49, Vicksburg MS, 1998.

Abstract:

MAGI is a smooth particle hydrodynamics (SPH) code currently in use by the Air Force to perform hypervelocity impact studies at the Air Force Research Laboratory (AFRL), Kirtland Air Force Base. In this report, we describe various approaches to parallelizing SPH as well as their current status. Four strategies for parallelizing MAGI are currently being investigated. There are two basic parallel programming models: shared memory and distributed memory. The shared memory approaches include SGI Power Fortran (PCF or OpenMP directives) and

Posix threads, whereas the distributed memory approaches include High Performance Fortran (HPF) and Message Passing Interface (MPI). We also make recommendations for further development.

98-50 Henry A. Gabb, "User Impact Study: CEWES MSRC CRAY C90 Decommissioning", CEWES MSRC/PET TR/98-50, Vicksburg MS, 1998.

Abstract:

The rationale for the decommissioning of the Cray C90 at CEWES MSRC is presented as well as the results from a user survey. The C90 is stated as being decommissioned due to high maintenance costs, poor price-to-performance ratio, and unsuitability for large high performance computing problems, which are becoming more prevalent. The results of the survey indicated that most users are already migrating or are interested in migrating to a parallel platform. The study reported that many of the custom codes running on the C90 can be migrated with no performance loss and usually a performance gain. Also, most of the commercial software is available in parallel versions. Thus, a successful migration of users is anticipated.

99-01 P. Baker, "What's New: A Report from SIGGRAPH98", CEWES MSRC/PET TR/99-01, Vicksburg MS, 1999.

Abstract:

SIGGRAPH98, the 25th meeting of the SIGGRAPH society, was recently held in Orlando. This is the major conference event for the computer graphics community. The conference offers an advanced technical program, a vendor exhibition of over 100,000 square feet, over 40 tutorial courses aimed at participants of various backgrounds, an interactive exhibit, and many other venues. This report summarizes the new technology shown at the conference.

99-02 R. Heiland and P. Baker, "A Survey of Coprocessing Systems", CEWES MSRC/PET TR/99-02, Vicksburg MS, 1999.

Abstract:

This report examines systems to support interactive computation, also known as computational monitoring and interactive steering. We review the existing software systems designed to support this capability.

99-03 Dongsoo Kang, Henry W. Park, Jinwoo Suh, Viktor K. Prasanna and Sharad N. Gavali, "Benchmarking of HPC Systems", CEWES MSRC/PET TR/99-03, Vicksburg MS, 1999.

Abstract:

High Performance Computing (HPC) platforms have gained widespread acceptance for meeting the computational requirements of large-scale applications. To evaluate the performance of these platforms, researchers have proposed various benchmarks. Some benchmarks attempt to measure the peak performance of these platforms by employing various optimizations and performance tuning to deliver close-to-peak performance. These benchmarks showcase the full capability of the products. However, for most users, these performance measures seem to be meaningless. For end-users, the actual performance depends on a number of factors including the architecture and the compiler used. Other benchmarks attempt to measure the performance of these platforms with a set of representative algorithms for a particular scientific domain. Although useful, these benchmarks do not give the end-users a simple method for evaluating their algorithms and implementations. We take a different view of benchmarking. Our benchmarks address the actual performance available to end-users. The benchmarks allow the end-users to understand the machine characteristics, the communication environment, and the compiler features of the underlying HPC platform at a user level. Using the results of our benchmarks, we attain our goal to provide end-users with a simple and accurate model of HPC platforms, including that of the software environment. Using such a model, end-users will be able to analyze and predict the performance of a given algorithm that allows algorithm designers to understand tradeoffs and make critical decisions to optimize their code on a given HPC platform. Our benchmarks provide the data and parameters necessary for the formulation of a model of HPC platforms. In predicting the performance of algorithms on HPC platforms, we assert that the key factor is accurate cost analysis of data access. Data may be communicated between memory and processor, between processors, or between secondary storage and processor. The possible locations of the data can be thought of as a data hierarchy. From our benchmarks, we formulated the Integrated Memory Hierarchy (IMH) model. The IMH model is a simple and accurate model able to predict the performance of data communication along the storage hierarchy. To demonstrate the accuracy and

usefulness of the IMH model, we have used it to predict the performance of the end-to-end program supplied to us by CEWES. We identified the major bottlenecks of the implementation and, using the IMH model, modified the parallelization of the code to improve scalability. Our implementation has been ported to the IBM SP, SGI/CRAY T3E, and Origin2000.

99-04 M. F. Wheeler, C. N. Dawson, J. Li and V. Parr, "UTPROJ: The University of Texas Projection Code for Computing Locally Conservative Velocity Fields", CEWES MSRC/PET TR/99-04, Vicksburg MS, 1999.

Abstract:

In the numerical modeling of fluid flow and transport problems, frequently the velocity field needs to be projected from one finite dimensional space into another. In certain applications, especially those involving modeling of multi-species transport, the new projected velocity field should be accurate as well as locally element-by-element mass conservative.

In this paper, a velocity projection method is developed that is both accurate and mass conservative cell-by-cell on the projected grid. The velocity correction is expressed as gradient of a scalar pressure field, and the resultant Poisson equation is solved using a mixed/hybrid, finite-element method and the lowest-order Raviart-Thomas spaces. Numerical results in two and three dimensions are presented.

99-05 R. Heiland and P. Baker, "Coprocessing: Experience with CUMULVS and pV3", CEWES MSRC/PET TR/99-05, Vicksburg MS, 1999.

Abstract:

This report describes our early experience with software packages that address the problem of interactive computation, or computational monitoring and steering. In particular, we describe the results of applying CUMULVS and pV3 to a parallel estuary modeling code.

99-06 S. Browne, G. Ho, and P. Mucci, "PAPI: Portable Interface to Hardware Performance Counters", CEWES MSRC/PET TR/99-06, Vicksburg MS, 1999.

Abstract:

The purpose of the PAPI project is to specify a standard application programming interface (API) for accessing hardware performance counters available on most modern microprocessors. These counters exist as a small set of registers that count Events, occurrences of specific signals related to the processor's function. Monitoring these events facilitates correlation between the structure of source/object code and the efficiency of the mapping of that code to the underlying architecture. This correlation has a variety of uses in performance analysis including hand tuning, compiler optimization, debugging, benchmarking, monitoring, and performance modeling.

PAPI provides two interfaces to the underlying counter hardware: A simple, high level interface for the acquisition of simple measurements and a fully programmable, low level interface directed towards users with more sophisticated needs. PAPI provides portability across different platforms. It uses the same routines with similar argument lists to control and access the counters for every architecture. As part of PAPI we have predefined a set of events that we feel represents the lowest common denominator of every good counter implementation. However, should the developer wish to access machine-specific events, the low level API provides access to all available events and counting modes.

99-07 A. Shih and P. Baker, "Management Strategies for Scientific Data: Assessing the Utility of HDF for CEWES MSRC Users", CEWES MSRC/PET TR/99-07, Vicksburg MS, 1999.

Abstract:

This paper review needs for data storage and management among high-performance computing users, particularly those at the CEWES MSRC. We also review the characteristics of the HDF file format package, with the intent of assessing its usefulness for MSRC users. Support packages for parallel I/O are also reviewed.

99-08 Wayne Mastin, "1998 CEWES MSRC PET Training Activities", CEWES MSRC/PET TR/99-08, Vicksburg MS, 1999.

Abstract:

This report contains a compilation of training activities of the CEWES MSRC PET program for January through December 1998. It includes a list of all training classes with attendance and evaluation figures, along with seminars, and distance education courses supported by the PET program.

99-09 J. White and S. W. Bova, "Where's the Overlap? An Analysis of Popular MPI Implementations", CEWES MSRC/PET TR/99-09, Vicksburg MS, 1999.

Abstract:

The MPI 1.1 definition includes routines for non blocking point-to-point communication that are intended to support the overlap of communication with computation. We describe two experiments that test the ability of MPI implementations to actually perform this overlap. One experiment tests synchronization overlap, and the other tests data-transfer overlap. We give results for vendor-supplied MPI implementations on the CRAY T3E, IBM SP, and SGI Origin2000 at the CEWES MSRC, along with results for MPICH on the T3E. All the implementations show full support for synchronization overlap. Conversely, none support data-transfer overlap at the level needed for significant performance improvement in our experiment. We suggest that programming for overlap may not be worthwhile for a broad class of parallel applications using many current MPI implementations.

99-10 Dan Nagle, "The Effect of Fortran 95 PURE and ELEMENTAL Procedures on Parallel Execution", CEWES MSRC/PET TR/99-10, Vicksburg MS, 1999.

Abstract:

The Fortran 95 statements, PURE and ELEMENTAL, are defined. These statements are already supported by many Fortran 90 compilers, including those at CEWES MSRC. The benefits of using PURE and ELEMENTAL functions are

discussed, as well as useful techniques to modify functions that are not PURE. Foremost among the benefits discussed is improved compiler optimization and parallelization. Several codes with side effects are presented along with equivalent, PURE, modified versions.

99-11 C. P. Breshears and G. Fagg, "A Computation Allocation Model for Distributed Computing under MPI_Connect", CEWES MSRC/PET TR/99-11, Vicksburg MS, 1999.

Abstract:

We present a modification to the standard Master-Worker model of dynamic, parallel task assignment. This new algorithm, dubbed the Queen-Drone model from the analogy of a multitude of drone bees working within several distinct hives under the direction of a single queen bee, is designed for use on distributed high performance platforms running under the MPI_Connect intercommunication library. Our modifications are straightforward and require only minor additions to existing codes written using the Master-Worker model. After describing our algorithm, we present some experiences and execution results of the Queen-Drone model applied to a simple integer factoring code and a large-scale harbor wave response code. We have been able to run experiments on machines of the same architecture, as well as between machines of different manufacture.

99-12 Mark R. Fahey and Dan Nagle, "Cray Fortran Pointers vs. Fortran 90 Pointers and Porting from the CRAY C90 to the SGI Origin2000", CEWES MSRC/PET TR/99-12, Vicksburg MS, 1999.

Abstract:

The differences between Cray Fortran pointers and Fortran 90 pointers are discussed along with important considerations when using Cray Fortran pointers on the SGI Origin2000. Issues when migrating code containing Cray Fortran pointers are discussed, including the effect of 64-bit compilation of Fortran 90 code containing Cray pointers. A discussion illustrating the differences between the pointer types is accomplished via the two-dimensional Fast Fourier Transform.

99-13 Dan Nagle, "The Benefits of Fortran Procedure Interfaces", CEWES MSRC/PET TR/99-13, Vicksburg MS, 1999.

Abstract:

The benefits of using procedure interfaces in Fortran code are discussed and examples of its use are presented. Some benefits discussed are: !) compilers can catch mistakes in arguments passed to a subprogram; 2) compiler optimizations may be more successful because the compiler is aware of the arguments that will be modified by subprograms; 3) interfaces enable users to write their own intrinsic functions; and 4) interfaces allow programmers to take advantage of operator and assignment overloading. Numerous examples of interfaces in various situations are presented.

99-14 G. C. Fox, W. Furmanski, S. Nair, H. T. Ozdemir, Z. Odcikin-Ozdemir and T. A. Pulikal, "WebHLA - An Interactive Multiplayer Environment for High Performance Distributed Modeling and Simulation", CEWES MSRC/PET TR/99-14, Vicksburg MS, 1999.

Abstract:

The process of integrating DoD Modeling and Simulation paradigms around the new HLA/RTI standards proceeds in parallel with the onset of new Object Web standards for distributed objects and componentware, emergent at the crossroads of CORBA-, DCOM-, Java-, and XML-based distributed object technologies. We describe here our WebHLA approach, which integrates both trends by offering Object Web-based implementation of the HLA framework. WebHLA follows a three-tier architecture including: a) Web / Commodity-based interactive simulation authoring and runtime front-ends given by Java applets or DirectX multiplayers; b) software bus in the middleware, given by Object Web RTI i.e. our implementation of DMSO RTI 1.3 as a Java CORBA service managed by JWORB (Java Object Web Request Broker); c) domain specific backend simulation modules, including advanced high performance DoD simulation kernels such as ModSAF or SPEEDES. We describe here the overall design of WebHLA, report on components prototyped so far, and summarize the status of the ongoing development of WebHLA applications.

99-15 G. C. Fox, W. Furmanski, G. Krishnamurthy, H. T. Ozdemir, Z. Odcikin-Ozdemir, T. A. Pulikal, K. Rangarajan and A. Sood, "Using WebHLA to Integrate HPC FMS Modules with Web/Commodity based Distributed Object Technologies of CORBA, Java, COM and XML", CEWES MSRC/PET TR/99-15, Vicksburg MS, 1999.

Abstract:

HLA standards for interoperability between various DoD Modeling and Simulation paradigms are being enforced in parallel with the rapid onset of new Object Web / Commodity standards for distributed objects and componentware, emergent at the crossroads of CORBA, COM, Java, and XML technologies. WebHLA explores synergies between and integrates both trends by offering Object Web-based implementation of the HLA framework. Our goal is to deliver a uniform platform that facilitates conversion of legacy codes to and development of new codes in compliance with HLA, HPC and Object Web standards. We outline the overall design of WebHLA, summarize the system components prototyped so far, and illustrate our approach for one HPC FMS application # Parallel CMS (Comprehensive Mine Simulator) — in the area of large scale minefield simulation and countermine engineering.

99-16 Tomasz Haupt, Erol Akarsu and Geoffrey C. Fox, "Landscape Management System: A WebFlow Application", CEWES MSRC/PET TR/99-16, Vicksburg MS, 1999.

Abstract:

This paper describes a pilot Web-based implementation of the Landscape Management System (LMS). The Web-based implementation extends the Watershed Modeling System by adding the capability to download the input data directly from the Internet, and execute the simulation codes on a remote high-performance host. This makes it possible to run LMS anywhere from a networked laptop. Furthermore, our system allows for constructing complex simulations by coupling several independently developed codes into a single, distributed application. The Web-based LMS is implemented as a WebFlow application. WebFlow is a modern three-tier commodity, standards-based, High Performance Distributed Computing (HPDC) system that integrates a high-level graphical user interface (Tier 1), distributed scalable object broker middleware (Tier 2), and a high-performance back end (Tier 3).

99-17 Benjamin Willhoite and Dan Nagle, "Using Fortran 90 Features for Cache Optimization", CEWES MSRC/PET TR/99-17, Vicksburg MS, 1999.

Abstract:

Several strategies for coding matrix operations in Fortran 90 are analyzed for their cache usage and resulting efficiency. In this report, a single algorithm is coded using five different cache blocking strategies. Each code is then compiled using four compiler optimization levels on both the SGI Origin2000 and the IBM SP. All versions of the code are tested and the results discussed.

99-18 Steve W. Bova, Clay P. Breshears, Christine Cuicchi, Zeki Demirbilek and Henry A. Gabb, "Dual-level Parallel Analysis of Harbor Wave Response Using MPI and OpenMP", CEWES MSRC/PET TR/99-18, Vicksburg MS, 1999.

Abstract:

It has become clear that the emerging class of high performance computers will have architectures based upon clusters of shared-memory processors (SMPs). The SGI/CRAY Origin2000 is an early example of this class which is currently available and offers non-uniform memory access (NUMA). Furthermore, IBM is reportedly developing a machine that will have small clusters of shared-memory processors connected via a message-passing network. The availability of Pentium-class motherboards that have four or more processors has also lead to relatively inexpensive machines of this type. It has recently become possible for high-performance applications to run on a network of multi-processor personal computers and communicate via the Message Passing Interface (MPI). A distinguishing characteristic of this architectural class is that it offers dual-mode parallelism: simultaneous shared and distributed-memory programming is possible. In order to exploit such architectures, however, research must be performed to identify and express nested parallelism within applications.

99-19 S. Kappes, "PET Web Pages Evolution", CEWES MSRC/PET TR/99-19, Vicksburg MS, 1999.

Abstract:

The CEWES PET web site serves as a communications medium for disseminating information to the HPC user community. Enhancements to this web site were required to facilitate the assimilation, sharing and dissemination of information resources across the CEWES MSRC PET user community, and to provide simplify generation and maintenance of the web site content. The existing CEWES PET web site was evaluated to identify enhancements required to improve information dissemination. Recommendations were provided that incorporate state-of-the-art web technologies to facilitate information exchange within and outside of the CEWES MSRC PET user community. Selected enhancements to the PET web site were then implemented to provide an improved design utilizing state-of-the-art functionality.

This report describes the new web site structure, how to migrate the old structure into the new design, and provides instructions for modifying navigation elements and utilizing Cascading Style Sheets to maintain visual consistency throughout the site.

99-20 O. Olatidoye, G. Jones, S. Sarathy, C. McIntyre, and L. Milligan, "Scientific Visualization for Interpretation and Assessment of Damage in Structures Subject to Blast Loads", CEWES MSRC/PET TR/99-20, Vicksburg MS, 1999.

Abstract:

There has been significant activity in the computational structural mechanics community, in developing methods to identify, and in assessing and predicting the effects of explosive blast loading on structures. The use of high performance computing tools in analysis and prediction of blast loading has provided an unprecedented insight and understanding on the mechanisms of failure, as well as methods to assess this damage in these cases. However, these analyses produce vast amounts of data, which are difficult to visualize. Researchers at Clark Atlanta University in collaboration with CEWES have developed a basic test bed to validate different visualization paradigms associated with different damage rules specifically for the visualization of blast analysis data. This paper outlines that framework and describes the approach adopted.

99-21 Troy Baer, David Ennis, James Giuliani, Leslie Southern and David E. Bernholdt, "Experiences with Using TANGO Interactive in a Distributed Workshop", CEWES MSRC/PET TR/99-21, Vicksburg MS, 1999.

Abstract:

Together, the Ohio Supercomputer Center (OSC) and the Northeast Parallel Applications Center (NPAC) at Syracuse University delivered high-performance computing (HPC) training courses to a geographically distributed Department of Defense (DoD) user community. In September of 1998, the Ohio Supercomputer Center (OSC) delivered a one-day offering on the Fortran 90 programming language from the CEWES MSRC in Vicksburg, Mississippi. In January of 1999, the OSC delivered a two-day offering on OpenMP from the CEWES MSRC. The TANGO Interactive collaborative software was used to deliver these courses simultaneously to participants at DoD HPC Modernization Program Major Shared Resource Centers and Distributed Centers. This report describes these prototype distance HPC courses, our experiences, and provides instructor and student guidelines.

99-22 D. J. S. Welsh, R. Wang, P. Sadayappan, and K. W. Bedford, "Coupling of Marine Circulation and Wind-Wave Models on Parallel Platforms", CEWES MSRC/PET TR/99-22, Vicksburg MS, 1999.

Abstract:

Accurate predictions of wave heights, currents, and water elevations are vital inputs in the planning of military operations in the marine environment. Marine circulation and wind-wave models have traditionally been run separately, but recent research has identified potentially important interactions between current and wave motions. This report details the coupling of the CH3D circulations model and the WAM wave model at the atmospheric boundary layer. The MPI parallel CH3D code and the OpenMP parallel WAM code have been coupled on the SGI Origin2000 at CEWES MSRC. Communication between the models is achieved using MPI, scalability results are presented for the individual codes and the coupled system, and results are included from hindcasts. The hindcasts show that wave-current interactions have a significant effect on storm surges and the associated currents. Work has also begun on the coupling of WAM and CH3D-SED, which includes the SED sediment transport model, at the bottom boundary layer. Details of the physics of this coupling are included in this report.

99-23 P. V. Bangalore, J. Zhu, D. H. Huddleston, A. Skjellum, D. J. S. Welsh, R. Wang, P. Sadayappan, and K. W. Bedford, "Development of a Scalable and Coupled Hydraulics and Sediment Model", CEWES MSRC/PET TR/99-23, Vicksburg MS, 1999.

Abstract:

The development of a fully coupled and scalable hydraulics, sediment, and wave model for simulation of physical marine processes has impact on many national defense and security operations. This report describes the development of a parallel version of a combined hydraulics and sediment model - a key component for the fully coupled model. The scalable version of the coupled hydraulics and sediment model was developed from the previously documented sequential version of the curvilinear hydrodynamics code in three dimensions with non-cohesive sediment transport (CH3D-SED). This report documents the development and verification of the parallel version of the coupled code. The parallel code was tested for two datasets on the CRAY T3E and Origin2000 at CEWES MSRC and performance results are presented.

99-24 Ray Burgess, "Year Four Focused Efforts", CEWES MSRC/PET TR/99-24, Vicksburg MS, 1999

Abstract:

This report describes the core support and focused efforts that were begun by the universities in support of the CEWES MSRC PET Program for year 4. New efforts that are added later in the year are not included. The report describes 28 efforts that support the areas of CFD, CSM, FMS, CSM, CWO, EQM, Tools, Training, Collaboration, and Scientific Visualization.

99-25 Ehtesham Hayder and John Mellor-Crummey "Improving Performance by Scalar Replacement in a CFD Code" CEWES MSRC/PET TR/99-25, Vicksburg MS, 1999.

Abstract:

We consider a moderate size computational fluid dynamics application code known as HELIX for a study of improving performance by scalar replacement, i.e., loading array element values that are used repeatedly into scalars to enable them to be register allocated by the back-end compiler. The goal of scalar replacement is to reduce load/store traffic.

Our experiments compare three versions of HELIX - the original code, a version in which scalar replacement was performed by hand, and version in which scalar replacement was performed automatically by Memoria - a tool for performing scalar replacement developed at Rice University and Michigan Technological University. Our experiments show that scalar replacement improves performance of this code by 4 to 12 percent over and above performance obtained by using the highest level of optimization with vendor-supplied compilers on an SGI Origin, an SGI O2 workstation, an IBM SP, and a CRAY T3E. Improvements in the execution time were primarily due to the reduction in the number of load/store instructions.

99-26 James B. White III, "Reading Sequential Unformatted CRAY C90 Files on an SGI Origin", CEWES MSRC/PET TR/99-26, Vicksburg MS, 1999.

Abtract:

The CRAY C90 and SGI Origin have different formats for the binary representation of Fortran data types, and they have different layouts for binary data in files. Therefore, a Fortran program compiled on an Origin cannot read a sequential unformatted file generated on a C90 without translating from the C90 file structure and data-type format. This document describes how to perform the required translation assuming only an Origin system is available.

99-27 M. Ehtesham Hayder, Constantinos S. Ierotheou, and David E. Keyes "Comparisons on an Archetypal PDE Computation", CEWES MSRC/PET TR/99-27, Vicksburg MS, 1999.

Abstract:

Three paradigms for distributed-memory parallel computation that free the application programmer from the details of message passing are compared for an archetypal structured scientific computation - a nonlinear, structured-grid partial

differential equation boundary value problem - using the same algorithm on the same hardware. All of the paradigms – parallel languages represented by the Portland Group's HPF, (semi-)automated serial-to-parallel source-to-source translation represented by CAPTools from the University of Greenwich, and parallel libraries represented by Argonne's PETSc - are found to be easy to use for this problem class, and all are reasonably effective in exploiting concurrency after a short learning curve. The level of involvement required by the application programmer under any paradigm includes specification of the data partitioning, corresponding to a geometrically simple decomposition of the domain of the PDE. Programming in SPMD style for the PETSc library requires writing only the routines that discretize the PDE and its Jacobian, managing subdomain-to-processor mappings (affine global-to-local index mappings), and interfacing to library solver routines. Programming for HPF requires a complete sequential implementation of the same algorithm as a starting point, introduction of concurrency through subdomain blocking (a task similar to the index mapping), and modest experimentation with rewriting loops to elucidate to the compiler the latent concurrency. Programming with CAP- Tools involves feeding the same sequential implementation to the CAPTools interactive parallelization system, and guiding the source-to-source code transformation by responding to various queries about quantities knowable only at runtime. Results representative of "the state of the practice" for a scaled sequence of structured grid problems are given on three of the most important contemporary high-performance platforms: the IBM SP, the SGI Origin 2000, and the CRAY T3E.

99-28 Chandrajit Bajaj and Steven Cutchin and Mary Wheeler, "Simulation Code Launching From The Web", CEWES MSRC/PET TR/99-28, Vicksburg MS, 1999.

Abstract:

Focussed effort two of the PET/CEWES project has been to develop web-based tools which serve as prototypes for launching parallel simulations from remote environments. The parallel simulations of interest arise in subsurface ow and transport, but the tools to be developed will be of general use. PARSSIM (Parallel Aquifer and Reservoir Simulator), a parallel, three-dimensional, ow and transport simulator for modeling contamination and remediation of soils and aquifers is being used in this demonstration. The code was developed at the University of Texas and contains many of the features of current state-of-the-art groundwater codes. It is fully parallelized using domain decomposition and MPI and is operational on the IBM-SP and CRAY T3E platforms.

99-29 Michael A. Chupa, Robert J. Moorhead "Oceanographic Model Visualization with the Interactive Structured Time-Varying Visualizer" (ISTV), CEWES MSRC/PET TR/99-29, Vicksburg MS, 1999.

Abstract:

The visualization of multigrid, multiresolution ocean models with the Mississippi State University ERC Interactive Structured Time-Varying Visualizer (ISTV) application is described as applied to a Wave Action Model (WAM) simulation of the 1998 El Nino event produced at the CEWES MSRC. Data manipulations required for visualization are described, along with development work in ISTV designed to provide built-in support for WAM visualizations. Other related ISTV work undertaken during contract year 3 is also discussed.

99-30 Dan Nagle and Joy Brogdon, "Fortran 90 Namelist I/O versus Cray Namelist I/O", CEWES MSRC/PET TR/99-30, Vicksburg MS, 1999

Abstract:

Migrating serial codes to parallel systems can be an intimidating endeavor. Compounding the programmer's apprehension may be the prospect of using Fortran 90 instead of Fortran 77. Fortran 90 standardized namelist input/output (I/O). Cray Fortran supported namelist as an extension prior to the Fortran 90 standard. There are some differences between the older Cray namelist and the Fortran 90 namelist. This report will discuss the most important differences. For a more complete description, the interested reader is referred to the Cray publication *Fortran Language Reference Manual, Volume 3* (publication number SR-3905, Edition 3.0, pages 93 et seq.).

99-31 Abani K. Patra, Atanas I. Pehlivanov, David Littlefield, Graham F. Carey, J. Tinsley Oden, "Application of Error Indicators and Local Adaptive Refinement for Elasto-Plastic Impact Calculation (EPIC)", CEWES MSRC/PET TR/99-31, Vicksburg MS, 1999

Abstract:

We have constructed extensions to the capabilities of the dynamic Lagrangian solid mechanics code EPIC ([10,11]) to enable basic h-adaptivity on a limited

range of problems. The indicators for adaptive refinement include a feature indicator based on relative velocity, a flux jump indicator, hybrid indicators an a stress recovery indicator. We use this capability to test different measures of solution quality and adaptive refinement schemes on a benchmark Taylor anvil test problem.

99-32 Geoffrey C. Fox, Roman Markowski, Nancy J. McCracken, Marek Podgorny, "More Experiences with TANGO Interactive in Synchronous Distance Learning Courses", CEWES MSRC/PET TR/99-32, Vicksburg MS, 1999

Abstract:

The Northeast Parallel Architectures Center at Syracuse University and the Computer Science Department at Jackson State University are now in their fourth semester of teaching computational science courses using the TANGO Interactive collaboratory system. All the course materials are on-line, and lectures are given twice a week in real time over the Internet. After the successful experience teaching undergraduates at JSU by faculty at SU in the first year, this report covers additional aspects of the teaching experience for graduate classes in the second year, additional improvements of technology for dealing with network bandwidth issues and teaching support, and the start of JSU faculty teaching a distance course at a third university.

99-33 Shirley Browne, Paul McMahan, Scott Wells, "Repository in a Box Toolkit for Software and Resource Sharing", CEWES MSRC/PET TR/99-33, Vicksburg MS, 1999

Abstract:

The Department of Defense High Performance Computing Modernization Program (HPCMP) seeks to bring technology to the warfighter. High performance software is being developed by the Common High-performance Software Support Initiative (CHSSI) component of the program. High-performance software and technology are being transferred to DoD users throughout he MSRC-supported Programming Environment and Training (PET) component. In any work environment, an individual's ability to perform his or her job is strengthened proportionally by the availability of the resources necessary to perform that job. The Repository in a Box (RIB) toolkit, developed by the University of Tennessee as part

of the federally funded National High-performance Software Exchange (NHSE) project, provides mechanisms for sharing software and other resources among and between DoD Computational Technology Areas (CTAs) and sites, thus helping to bring this technology to the warfighter. RIB has been used to set up a distributed collection of interoperable software repositories for the DoD Major Shared Resource Centers (MSRCs). This network of repositories allows software, algorithms, and experiences to be shared within and between TAs and MSRCs as well as with the broader DoD user community. Use of RIB provides a uniform and consistent user interface to these repositories. Extensions to the basic RIB data model are allowing value-added information, such as software evaluations, performance studies, deployment information, and intellectual property rights, to be cataloged. Thus RIB allows all pertinent information about the software to be consistently maintained and accessed from the same interface. Moreover, RIB enables DoD users to leverage other HPC efforts, such as NASA HPCC and NSF PACI, that are also using RIB to make resources developed by their programs available to users. This report gives an overview of the functionality of RIB, describes current DoD RIB repositories, and concludes with future plans.

Team Member	Affiliation	Location	ocation Title Role		% Time	Days On-Site
		ERC (Mi	ssissippi State) - LEADERSHI	P		
Joe Thompson, Ph.D.	MSU	At University	Distinguished Professor	Academic Team Lead	61	77
		ERG	C (Mississippi State) - CFD			
David Huddleston, Ph.D.		At University	Associate Professor	CFD Academic Lead	12	5
Steve Bova, Ph.D.		On-site	Research Engineer	CFD On-Site Lead	100	All
Jianpiang Zhu, Ph.D.	MSU		Professor		14	0
Puri Bangalore		At University	Research Assistant	CFD Code Parallelization	50	10
		TICAM (Texa	as) & ERC (Mississippi State) -	· CSM		
J. Tinsley Oden, Ph.D.	_		Professor, TICAM Director		10	5
Graham Carey, Ph.D.	Texas	At University	Professor	CSM Academic Co-Lead	15	6
Rick Weed, Ph.D.	MSU	On-Site		CSM On-Site Lead	100	All
David Littlefield, Ph.D.					50	3
Atanas Pehlivanov, Ph.D.	Texas		Research Engineer	CSM Code Optimization	50	0
Robert McLay, Ph.D.		At University		Software Specialist	50	0
Abani Patra, Ph.D.	University of Buffalo		Assistant Professor	CSM Code Optimization	12.5	0

Table 1
TECHNICAL SUPPORT TEAM PERSONNEL

Team Member	Affiliation	Location	Title Role		% Time	Days On-Site
			Ohio State - CWO			
Keith Bedford, Ph.D.			Professor	CWO Academic C0-Lead	10	2
Ponnuswamy Sadayappan, Ph.D.		At University	Professor	CWO Academic Co-Lead	15	8
Stephen Wornom, Ph.D.		On-Site	Senior Research Scientist	CWO On-Site Lead	100 (1/99 - 3/99)	All
Shuxia Zhang, Ph.D.	Ohio State	Ohio State	Research Scientist	CH3D-SED support, model coupling	100 (4/98 - 9/98)	0
David Welsh, Ph.D.		At University	Senior Research Associate - Engineer	WAM and CH3D support, model coupling	100	31
Rong Wang			Graduate Research Associate	Code Parallelization, model coupling	100 (10/98 - 3/99)	0
		,	TICAM (Texas) - EQM			
Mary F. Wheeler, Ph.D.			Professor	EQM Academic Lead	8.5	7
Clint N. Dawson, Ph.D.		At University Texas	Associate Professor	Training, Projection and Advection, Parallel Migration	12.75	2
Victor Parr, Ph.D.	Texas		Research Associate	Parallel Migration, Code Development, Tutorials	90	18
Robert Fithen, Ph.D.		On-Site	Research Associate	EQM On-Site Lead	100 (4/98 - 6/98)	All

Table 1
TECHNICAL SUPPORT TEAM PERSONNEL

	_					
Team Member	Affiliation	Location	Title	Role	% Time	Days On-Site
Monica Martinez-Canales, Ph.D.			Postdoctoral Fellow	Outreach, Tutorials, Parallel Migration	17	2
Jichun Li, Ph.D.	Texas	At University	Research Associate	Development of UTPROJ3D, Parallel Migration	34	0
Steve Bryant, Ph.D.		At Offiversity	Research Associate	Web Launching, Parallel Migration	34	0
Steve Cuchins			Graduate Student	Web Launching	10	0
Robert Kirby			Graduate Student	Web Launching	10	0
		NPA	AC (Syracuse) - FMS & C/C			
LEADERSHIP (0.39 FTE)		Professor	NPAC Academic Lead		3
David Bernholdt, Ph.D.	Syracuse	At University	Senior Research Scientist	Project Leader		2
CANGO INTERACTIVE	COLLABORAT	ΓORY GROUP (2.9				_
Marek Podgorny, Ph.D.			Senior Research Scientist	Project Leader		2
Greg Lewandowski	C	A A I I I I I I I I I I I I I I I I I I				0
Tom Major	Syracuse	At University	Research Scientist	Research Scientist		0
Konrad Olsweski						0

Table 1

	1		SUPPORT TEAM PER			
Team Member	Affiliation	Location	Title	Role	% Time	Days On-Site
Pawel Roman						0
Piotr Sokolowski						0
Tom Stachowiak			Research Scientist	Research Scientist		0
Remek Trzaska	g	Cacuse At University Graduate Research Scientist				2
Bart Winnowicz	Syracuse					0
Luke Beca					0	
Dongmin Kim			Graduate Research Scientist	Graduate Research Scientist		0
Norka Lucena				belendst		0
NTERACTIVE WEB TE	ECHNOLOGIES	GROUP (3.04 FTI	Ε)			
Wojtek Furmanksi, Ph.D.			Senior Research Scientist	Project Leader		0
Tom Haupt, Ph.D.			Schol Research Scientist	riojeci Leauei		18
Erol Akarsu						0
Harish Dhingra		A. TT				0
	Syracuse	At University				

Erol Akarsu		
Harish Dhingra	a a	A . TT
Survesh Jithendran	Syracuse	At University

0 Graduate Research Graduate Research Assistant Assistant 0 0 0

Dinesh Kasthuril

Ganesh Krishnamurthy

Hasan Ozdemir

Team Member	Affiliation	Location	Title	Role	% Time	Days On-Site
Zeynep Ozdemir						0
Tom Pulikal						0
Krishnan Rangarajan		acuse At University	Graduate Research Assistant	Graduate Research Assistant		0
Sachin Shanbhag	Syracuse					0
Anusha Shankar						0
Rudrasen Shitole						0
Ankur Snood						0

COMPUTATIONAL SCIENCE EDUCATION GROUP (0.45 FTE)

Nancy McCracken, Ph.D.			Semior Research Scientist	Project Leader	0
Ozgur Balsoy	Syracuse				0
Saleh Elmohamed			Graduate Research Assistant	Graduate Research Assistant	0
Meyrem Ispirli		Syracuse At University		- 15515 1411	0
Deepak Ramanathan			Computer Consultant	Computer Consultant	0
Mehmet Sen			Graduate Research Assistant	Graduate Research Assistant	0

Team Member	Affiliation	Location	Title Role		% Time	Days On-Site
DATABASE APPLICAT	IONS GROUP (().33 FTE)				
Chao-Wei Ou, Ph.D.	G	A 4 TTu:	Daniel Grinder	December Scientist		0
Yuping Zhu	Syracuse	At University	Research Scientist	Research Scientist		0
		CRP	PC (Rice, Tennessee) - SPPT			
Ken Kennedy, Ph.D.		At University	Professor	SPPT Senior Academic Lead	4	0
Charles Koelbel, Ph.D.			/	SPPT Academic Lead	25% (4/98 - 7/98))	3
Clay P. Breshears, Ph.D.		On-site	Research Scientist	SPPT On-Site Lead	100	All
Dick Hanson, Ph.D.	Rice			SSPT Academic Lead	75% (1/99 - 3/99)	3
Gina Goff, Ph.D.				Software Analyst	25% (Left position on 12-31-98)	2
Ehtesham Hayder, Ph.D.		At University		Research Scientist II	33	7
Shirley Browne, Ph.D.	Tennessee		Associate Research Director of ICL	Interactive Performance Analysis and Debugging Interoperable CTA Repositories	39	6
Graham Fagg, Ph.D.	Tennessee		Research Asst. Professor	MPI_Connect	14	5

Table 1
TECHNICAL SUPPORT TEAM PERSONNEL

Team Member	Affiliation	Location	Title	Title Role		Days On-Site
George Ho	Tennessee		Graduate Student	Interactive Performance Analysis and Debugging	18	0
Kevin London	Tennessee		Research Associate	Interactive Performance Analysis and Debugging, MPI Connect	31	2
Paul McMahan	Tennessee		Program Director	Interoperable CTA Repositories	20	0
Phil Mucci	Tennessee	At University	Research Consultant	Interactive Performance Analysis and Debugging	25	0
Martin Swany	Tennessee		Research Associate	MPI_Connect	8	0
John Thurman	Tennessee		Graduate Student	Interactive Performance Analysis and Debugging	25	0
Scott Wells	Tennessee		Program Director	Interoperable CTA Repositories	10	0
		NCSA (Illin	ois) & ERC (Mississippi State)	- SV		
Polly Baker, Ph.D.			Associate Director	SV Academic Lead	20	8
Alan Shih, Ph.D.			Research Scientist	NCSA SV Site Lead	100	75
Dave Bock	NCSA	At University			25	3
Randy Heiland			Research Programmer	Project Developer	25	5
Rob Stein					25	0

Table 1
TECHNICAL SUPPORT TEAM PERSONNEL

Team Member	Affiliation	Location	Title	Role	% Time	Days On-Site
Robert Moorhead, Ph.D.			Professor	Project Director	0	5
Michael Chupa					37	4
Kelli McCarter			Research Assistant I	Project Developer	29	2
Cass Everitt					0	2
Brandon Butler					2	0
Wai-Tat Wong	MSU	At University	iversity Student	_	2	0
Derek Irby				Programmer	2	0
Gene Hellums					2	0
Raghu Machiraju Ph.D.			Assistant Professor	Project Director	20	6
Balakrishna Nakshatrala			Graduate Research Assistant	Project developer	25	0
		Jacks	son State University (HBCU)			
Willie G. Brown, Ph.D.			Assistant Vice President for Information Technology	HBCU/MI Lead, JSU Lead	10	10
Mildred Leonard	7077		Scientific Visualization Specialist	Scientific Visualization Support	100	10
Michael Robinson	JSU At University	Network Training Specialist	Distance Education Technical Lead	100	0	
Edgar Powell			Scientific Visualization Technician	Scientific Visualization Support	100	10

Team Member	Affiliation	Location	Title Role		% Time	Days On-Site	
	University of Southern California						
Viktor K. Prasanna, Ph.D.			Professor	USC Lead	10	4	
Henry Park					50	4	
Jinwoo Suh	USC	At University		Performance	50	0	
Dongsoo Kang			Graduate Research Assistant	Benchmarking and Modeling	50	0	
Myungho Lee					50	0	
		(Clark Atlanta University				
Olu. Olatidoye, Ph.D.	CAU	At University	Principal Investigator (PI)	CAU-MSRC CSM-PI/Analyst/Structural Engineer	3	4	
Gary Jones			Research Engineer	Programmer/Structural Engineer	100	23	
Eddie Mason			Student	24.11	17	0	
Clauzel McIntyre			Graduate Student	Programmer/Modeling	0	0	
Leon Milligan			Student	Modeling/Simulation	67	0	
SriPrakash Sarathy, Ph.D.			Professor of Engineering	Co-Investigator, Simulation	11	0	

This page intentionally left blank

Table 2 TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose				
	ERC (Mississippi State) - Leadership							
			1					
			1					
CEWES			4	On-Site Leadership				
			1					
			1					
Wash D.C.		MSU Thompson	1	DoD Meeting				
			1					
			2					
	MSU		1					
			2					
			2					
CEWES			1	On-Site Leadership				
			4					
			1					
			1					
			2					
CEWES	MSU		2	On-Site Leadership				

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
CEWES			2	On-Site Leadership
Houston, TX			6	DoDHPCMP Users Group Conference
	MSU	Thompson	3	
CEWES			2	On-Site Leadership
			2	
	EI	RC (Mississippi State) - CFD		
CEWES MSRC		Huddleston	2	CEWES MSRC Pet Annual Review
Jackson State			1	Jackson State HPC Summer Institute (presenter)
Jackson State			1	Give seminar
Rice			5	DoD HPCMP User Group Meeting (presenter)
ONR Wash D.C.	MSU	Bova	4	22nd Symposium on Naval Hydrodynamics
Mississippi State			2	ERC Industrial Affiliates Meeting
Orlando FL			6	SC98 (presenter)
NRL			2	MPI Tutorial (instructor)
Jackson State		Zhu	1	Jackson State HPC Summer Institute (presenter)

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
Memphis TN		Zhu	4	ASCE Water Resources Conference (presenter)
Ohio State			4	OSU Collaboration
NRL			3	MPI Tutorial (instructor)
CEWES MSRC			2	Technical Contacts
CEWES MSRC	MSU	Bangalore	3	MPI Tutorial (instructor)
CEWES MSRC			2	OpenMP Short Course
NRL			2	MPI Tutorial (instructor)
CEWES MSRC			4	MPI Tutorial (instructor)
Jackson State		Berg	1	Give seminar
	TICAM (Te	exas) & ERC (Mississippi State	e) - CSM	
Rice		Carey	1	DoD HPCMP User Group Meeting (short course)
CEWES MSRC	T	Carey, Oden	2	CSM Workshop (presenters)
Sandia	Texas	Littlefield	1	Collaboration on CTH
		Carey + student	2	Collaboration on unstructured grid partitioning, discuss transfer of CHACO

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose	
University of Buffalo		Pehlivanov	1 week	Collaboration with Patra on indicator modules for EPIC	
University of Texas	Texas	Patra	1 week	Collaboration with Pehlivanov on EPIC and Littlefield on CTH.	
CEWES MSRC		Carey, Oden, Littlefield	3	CEWES MSRC PET Annual Review	
Eglin AFB			1	Parallel EPIC Review	
UT Austin			1	Coordination meeting for CSM Core Support and FE	
Rice			6	Users Group Meeting	
UT Austin	MSU		1	Mid-Year Review Presentation	
Clark Atlanta University			Dr. Rick Weed	1	Coordination Meeting
UT Austin			1	EQM Mid-Year Presentation Coordination Meeting	
Groton, CT			4	Presented Parallel Fortran Programming Workshop	
Eglin AFB			1	Parallel EPIC Final Program Review	
Austin/San Antonio		Dr. Rick Weed	4	San Antonio TX TICAM/ SIAM Parallel Programming Conference at San Antonio	

Table 2 TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose			
Ohio State - CWO							
Mississippi State		Sadayappan, Zhang	1	CH3D-SED and model coupling withBilly Johnson and Puri Bangalore			
CEWIES MSD.C		Sadayappan	2	WAM with Bob Jensen, Carol Beaty, Don Resio, and Linwood Vincent; PET video for the ITL Open House with Strelitz			
CEWES MSRC	CEWES MSRC	Welsh	4	WAM with Bob Jensen, Carol Beaty, Don Resio, and Linwood Vincent; PET video for the ITL Open House with Strelitz			
Rice		Welsh	4	Dan HDCMD Haar Cross Marking			
Rice	Ohio State	Sadayappan	2	DoD HPCMP User Group Meeting			
Jackson State		Bedford, Sadayappan, Zhang, Welsh	2	Jackson State HPC Summer Institute (presenters)			
		Welsh	3	WAM with Bob Jensen, Carol Beaty, and			
CEWES MSRC		Sadayappan	2	Alex Carillo			
		Welsh	4	CEWES MSRC PET Midyear Review and CWO Core Support			
		Welsh	5	WAM with Bob Jensen, Alex Carillo, and			
		Sadayappan	2	Trey White			

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
		Welsh	5	CWO Core Support with Bob Jensen and Henry Gabb
CEMES WODG		VV CISII	5	CWO Core Support with Bob Jensen
CEWES MSRC	Ohio State	Bedford, Sadayappan	2	CEWES MSRC PET Annual Review
		Welsh	5	CEWES MSRC PET Annual Review and CWO Core Support
Mississippi State		Wornom	1	CWO issues with Huddleston, Zhu, Moorhead, and Joe McCaffrey
		TICAM (Texas) - EQM		
Texas	University of		3	
	New Orleans		3	Interview for On-Site Lead
CEWES MSRC Jackson State		Wheeler	3	Jackson State HPC Summer Institute and discussions with CEWES EQM researchers
D:			1	DoD HPCMP User Group Meeting
Rice	Rice Texas	Dawson	2	(presenter)
In Law Contra		Lozano	2	Jackson State HPC Summer Institute
Jackson State		Martinez	2	(presenter)
_		Fithen	4	PROFEM
Texas	Stanford	Martinez	4	ADCIRC

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose	
Orlando FL		XXII 1	3	SC98	
GEWEG MGD C	Texas	Wheeler	3		
CEWES MSRC		Dawson	3	Workshop on parallel techniques	
UT Austin	NAVO	Luong	3	Interview for EQM On-Site Lead	
CENTER WODE	Texas	Wheeler	3	CEWES PET Annual Review	
CEWES MSRC	NAVO	Luong	3	Interview for EQM On-Site Lead	
CEWES MSRC	UT Austin		8		
Orlando, FL		UT Austin	D. D.	4	REMARK: Parr made 16 trips to CEWES
Rice			UT Austin	Parr	5
Texas			12		
	NI	PAC (Syracuse) - FMS & C/C			
GEWEG MOD G		Haupt	1	Deliver Web Information Training	
CEWES MSRC		Bernholdt, Fox	2	CEWES MSRC PET Annual Review	
Jackson State	Syracuse	McCracken	1	Distance Course Final Projects	
CEWES MSRC		Podgorny, Trzaska	2	Tango Interactive Training class	
Orlando FL		Fox, Haupt, McCracken, Ozdemir, Ozdemir,Podgorny	6	SC98 Demonstrations & presentations of CEWES MSRC-supported work	

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
			17	Work with LMS Group (lead by Jeff Holland)
CEWES MSRC		Haupt	5	Work with LMS Group (lead by Jeff Holland)
			1	CEWES MSRC PET Mid-Year Review
Jackson State		Fox	1	Distance Course Check-up
Jackson State		Podgorny, Stachowiak, Lewandowski	3	Tango Setup and Ttraining
CEWES MSRC	Syracuse	Haupt	2	Work with LMS Group (lead by Jeff Holland)
University of Texas		Haupt	1	Meeting with Mary Wheeler's Group
Jackson State		Furmanski, Nair, Pulikal	2	FMS Lecture & Lab at Jackson State Summer Inst.
CEWES MSRC		Haupt	1	Work with LMS Group (lead by Jeff Holland)
			3	Deliver Java Training
		McCracken	2	Distance Course Final Projects
	CF	RPC (Rice, Tennessee) - SPPT		

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
		Koelbel	1	Consult with PET team
		Goff, Hayder, Koelbel	2	Taught tutorial at CEWES MSRC
CEWES MSRC		Hayder	2	Attended CSM HPC workshop
		Hanson, Hayder	1	Consult with On-Site SPPT Lead
		Hanson, Hayder	2	CEWES MSRC PET Annual Review
NCSA	Rice	Breshears	2	Meet with NCSA Virtue team
Rice	RICE	Breshears	5	DoD HPCMP Users Group Meeting (presenter)
Rice		Breshears	3	Tutoring session at Rice
Boulder CO		Breshears, Goff	2	Parallel Tools Consortium Annual Meeting
Denver CO		Hayder	3	CUG O2K workshop
NRL		Goff , Hayder, Koelbel	2	Taught tutorial at NRL
Orlando FL	Rice	Breshears, Hayder	6	SC98; Breshears participated in HPC Challenge
Tennessee	Rice		2	Meet with Browne for CEWES MSRC PET Mid-Year Review material
University of Southern Mississippi	Rice Rice	Breshears	3	First Southern Conference on Computing
San Diego CA			5	IBM SP Advanced Computing Technology Scientific Applications Development and Optimization Meeting (presenter)

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
Pittsburgh PA	Rice	W - 11 - 1	3	LCRS workshop
Orlando FL	Rice	Koelbel	2	SC98
Boulder CO		Browne	5	Parallel Tools Consortium Annual Meeting
		London	4	
Rice		Mucci, Brown, Blackford	5	DoD HPCMP Users Group Meeting
		McMahan	3	
Ohio State		Fagg	2	Collaborate with OSU CWO team
Los Alamos			5	Collaborate with DoE ASCI Parallel Tools Team
Denver CO		Browne	4	Cray Users Group - Origin 2000 Workshop
Timberline OR	Tennessee		4	Parallel Tools Consortium Steering Committee Meeting
any na 1, an a		Browne	3	Collaborate with On-Site SPPT Lead
CEWES MSRC		Fagg	4	Collaborate with on-site staff
Orlando FL		Fagg, London	6	SC98
Orlando FL		Browne	4	SC98
		Browne	3	Teach TotalView/Vampir training course
CEWES MSRC		London	3	Work with on-site systems staff
Poughkeepsie NY		Browne, London	2	Meet with IBM DPCL team

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
NCSA	Tennessee	Browne, London	3	Meet with NCSA Virtue team
San Diego CA	Tennessee	Browne	3	Parallel Tools Consortium Steering Committee Meeting
CEWES MSRC	Tennessee	Browne, Fagg	3	CEWES MSRC PET Annual Review
	NCSA (Illi	nois) & ERC (Mississippi State	e) - SV	
		Baker, Shih	4	CEWES MSRC PET Annual Review
		Baker, Bock, Heiland	3	Technology Transfer
CEWES MSRC	NCSA	Heiland, Semeraro	2	D. I
		Folk	2	Deliver Training
		Shih	75	User contact, planning
Berkeley CA		Baker	4	DOE Vis workshop
Orlando FL		Baker, Bock, Shih, Stein	6	Graphics conference
Orlando FL		Baker, Bock, Heiland, Shih	6	SC98
North Carolina	NCSA	Baker, Stein	6	IEEE Vis conference
Rice		Baker, Shih, Heiland	5	DoD HPCMP User Group Meeting
ASC MSRC		Shih	2	Consulting & Training
ARL MSRC		Baker, Bock, Heiland, Shih	4	DoD Vis workshop

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
CEWES MSRC		Moorhead, Chupa, Everitt, McCarter	1	Overview of MSU vis capabilities
NRL/SSC		Chupa	2	Learn how to help NLOM personnel and work with them.
		Moorhead, Chupa, Everitt, McCarter	1	Meet with Jensen's ocean modeling group
	MSU	Moorhead, Chupa	1	Deliver ISTV course
CEWES MSRC		Moorhead	2	CEWES MSRC PET Annual Review
OD WED MAKE		Chupa	1	Attend WebFlow training & meet with ocean modeling group
		Machiraju	1	Interactions with CSM users at CEWES MSRC
Orlando FL		Machiraju	1	Siggraph 98
Research Triangle Park, NC	MSU	Machiraju	2	Visualization 98
		Jackson State		
Dayton, OH		Brown	2	Meeting with Lisa Burns at ASC MSRC
Jackson, MS		Brown, Leonard, McClinton, Moore, Robinson, Wicks	2	Annual Creating Futures through Technology Conference
CEWES MSRC	Jackson State	Brown, Leonard, McClinton, Moore, Robinson, Wicks	2	CEWES MSRC PET Annual Review Meeting
Mississippi State		Powell	1	Meeting with Robert Morehead

Table 2
TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose
Syracuse		Robinson	2	Attend training session at Syracuse
Baltimore MD		Robinson	4	Travel to Morgan State and assist in set-up of a computer course
O look FI		Leonard	5	0,000
Orlando FL		Brown	5	SC98
CEWES MSRC		Leonard	1	DoD High performance computing
CEWES MSRC	Jackson State	Leonard	1	consultation
Mississippi State		Powell	1	To attend a meeting and planning to set up training at MSU
Atlanta GA			2	PET Retreat
Rice		Brown	2	DoD HPCMP Users Group Meeting at Rice
ASC MSRC			3	PET Group Meeting
NCSA		Powell, Leonard	5	Alliance 98 Conference at NCSA
	Univ	versity of Southern California		
		Park	2	CEWES MSD C DET M' L V D. ' .
CEWES MSRC	USC	Prasanna	2	CEWES MSRC PET Mid-Year Review
		Park	2	CEWES MSRC PET Annual Review

Table 2 TEAM TRAVEL

Destination	Institution	PET Personnel	Duration Days	Purpose					
Clark Atlanta University									
CEWES MSRC	CAU	Jones	26	One-on-one work on Damaged Structures project with Dr. Raju Namburu.					
		Olatidoye	1	Attend CoMET presentation					
		Jones	2	Attend Mid-Year Review					
		Jones, Olatidoye	4	To attend CEWES meeting					
Orlando, FL		Milligan	6	To attend Siggraph '98 Conference					
CEWES MSRC		Olatidoye	2	Attend Annual Review					

Table 3 CEWES USER CONTACTS

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Don Kenzakowski	NASA Ames				Training/collaboration
Marty Moulton	NASA Ames	CFD		T. 1. 1	
Alan Wallcraft	NRL Stennis			Telephone	Training
Matt O'Keefe	AHPCRC	CWO			Outreach
Chao-Ho Sung	David Taylor Model Basin	CFD	MSU: Bova	E-mail	
Zeki Demirbilek		CFD/EQM		Visit/phone/E-mail	
Charlie Berger		CFD		Visit to ERC	Training/collaboration
Bob Bernard	CEWES				
Billy Johnson					
Norm Scheffner					
Raju Namburu	CEWES	gg) (Texas: Carey/Oden/Littlefield	Phone, E-mail, visits	CSM workshop, CTH application, UT Adaptive Workshop, Adaptive CTH
Mark Adley, Steve Akers	CEWES	CSM	Weed	Visit	Nonlinear material modules, parallel needs, adaptive contributions
Kent Kimsey, Dan Scheffler, David Kleponis	ARL	CSM	Texas:Littlefield	Phone, visits	Application discussions

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Raju Namburu		CSM	CAU:Olatidoye		Research Interaction/Review meetings/Sucess Stories
All	CEWES	CSM, CFD, Tools, FMS, EQM, SciVis	Baskervile-Lottie	Phone, E-mails, visits	High Performance Computing Application and Technology (HiPCAT) Conference
Bob Jensen, Alex Carillo		CWO	OSU: Welsh		Sent copies of OSU bi-weekly reports
Jeff Holland		CWO/EQM	OSU: Welsh		Sent copies of OSU bi-weekly reports
Bob Jensen, Christine Cuicchi	CEWES		OSU: Sadayappan, Welsh	E-mails	Exchanged e-mails regarding testing of MPI WAM on CEWES platforms
D. l. J		CWO	M OSU: Welsh OSU: Sadayappan, Welsh	Reported that sign errors had been found in WAM propagation subroutine	
Bob Jensen			OSU: Welsh		Planned on-site WAM co-ordination meeting for 5/98
Billy Johnson			OSU: Sadayappan, Zhang	Meeting at MSU	Discussed CH3D and CH3D-SED activities

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Bob Jensen			OSU: Sadayappan, Welsh	On-site meeting	WAM activities co-ordination meeting in 5/98 with Jensen, and Beaty of SGI
			OSU: Welsh		Sent corrected WAM propagation subroutine
Bob Jensen, Christine Cuicchi			OSU: Weish		Sent trip report for CEWES visit in 5/98.
					Sent CH3D-SED plots requested by Johnson
Billy Johnson	CEWES	CWO	OSU: Zhang	E-mails	Reported the effects of compilation arguments on CH3D results, an investigation requested by Johnson
Jay Shriver			OSU:Welsh		Welsh asked Shriver about the scalability of data assimilation techniques he is using
Bob Jensen, Christine Cuicchi			OCU, Cadamana Walah		Discussion of differences found between MPI WAM and sequential WAM results
Bob Jensen			OSU: Sadayappan, Welsh		Planned on-site WAM co-ordination meeting for 8/98

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT		
Bob Jensen, Christine Cuicchi				E-mails	Discussion of debugging of MPI WAM errors		
Bob Jensen, Alex Carrillo			OSU: Sadayappan, Welsh	On-site meeting	WAM activities co-ordination meeting in 8/98 with Jensen, Carillo, and Beaty of SGI		
Bob Jensen, Christine Cuicchi, Alex Carrillo			OSU: Sadayappan	E-mails	Sent trip report for CEWES visit in 8/98		
Bob Jensen, Christine Cuicchi, Alex Carrillo		CWO	CWO	CWO	OSU: Sadayappan, Welsh	E-mails and phone	Worked on document for PET management detailing MPI WAM problems and alternative strategies for continuing WAM efforts
Bob Jensen, Alex Carrillo	CEWES				OCH W.L.		Reached agreement to replace MPI WAM with OpenMP WAM
Bob Jensen					OSU: Welsh	E-mails	Planned on-site WAM co-ordination meeting for 10/98
Bob Jensen			OSU: Sadayappan, Welsh	On-site meeting	WAM activities co-ordination meeting in 10/98		
Bob Jensen			OSU: Welsh	E-mails	Notified Jensen of ftp site for latest release of the WAM model		
Bob Jensen, Alex Carrillo					Sent trip report for CEWES visit in 10/98		

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
				E-mails	Exchanged updates on debugging of OpenMP WAM
Bob Jensen			On-site meetings OSU: Welsh	Update meetings during CWO Core Support trips	
		CWO		E-mails	Sent Jensen preliminary CWO training course announcement which he sent to CEWES CHL mailing list
Lori Hadley			OSU: Wornom	On-site meeting	Discussed Hadley's use of the SWAN code
Jeff Holland	CEWES	CWO/EQM		On-site meeting	Met to discuss CH3D/WAM coupling and CWO training class
Bob Jensen		CWO	OSU: Welsh	E-mails	Notified Jensen of abnormal WAM run terminations when currents are included and grid is not divided into blocks
Bob Jensen					Wornom introduced himself
Joe Gailani			OSU: Wornom	Telephone call	as the new CWO On-Site
Jeff Holland		CWO/EQM			Lead

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT		
Billy Johnson							
Norm Scheffner				Telephone call	Wornom introduced himself as the new CWO On-Site		
Nicolas Kraus	CEWES	CWO	OSU: Wornom	reiephone can	Lead		
Zeki Demirbilek							
Bob Jensen, Joe Gailani				On-site meeting	Discussed PET Year 4 CWO priorities		
Lori Hadley			CWO		OSU: Wornom	Telephone call	Wornom introduced himself as the new CWO On-Site Lead
Bob Jensen					OSU: Welsh	E-mails	Discussed plans for a CWO co-ordination meeting at NAVOCEANO/NRL Stennis
Lori Hadley	CEWES			OCH W.	Telephone call	Discussed Hadley's use of the SWAN code, and the migration of SWAN to parallel platforms	
Zeki Demirbilek			OSU: Wornom	On-site meeting	Wornom discussed CGWAVE activities with Demirbilek and Gabb of CMG		
Jeff Holland		CWO/EQM	OSU: Bedford, Welsh	E-mails	Holland requested and received information concerning future CH3D-SED plans		

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Zeki Demirbilek		CWO/SV		On-site meeting	Wornom discussed CGWAVE graphics needs with Demirbilek and Strelitz of SV
			OSU: Wornom Texas Mary Wheeler, Clint Dawson, Victor Parr	Telephone call	Discussed graphics needs for the SWAN model
Lori Hadley	CEWES	CWO		On-site meeting	Wornom discussed the migration of SWAN to parallel platforms with Hadley, Jensen, Gabb and Willhoite of CMG, and Breshears of SPP Tools
Carl Cerco					Code requirements for EPA scenarios
Jeff Holland		EQM		Office visits, calls, E-mails	Discuss PET EQM projects
Mark Dortch			,		Technology transfer to CE-QUAL-ICM/TOXI
Tim Madden	AFRL Phillips Lab	Modeling	Texas Clint Dawson	E-mail	Information on domain decomposition techniques
Barry Bunch				Office visits, calls, E-mails	Code requirements for EPA scenarios
Mark Noel	CEWES	EQM	Texas Victor Parr	Office visits, calls, E-mails	Training for use of parallel CE-QUAL-ICM, joint talk at DoD User's Meeting June 1998

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT					
Terry Gerald				065.	Training how to parallelize CE-QUAL-ICM/TOXI					
Ross Hall			Texas Victor Parr	Office visits, calls,	Training how to parallelize CE-QUAL-ICM/TOXI					
Rao Vemulakunda	CEWES	EQM	EQM	EQM	EQM	EQM	EQM		Office visit	Code requirements for parallel ADCIRC
Charlie Berger			Texas Victor Parr, Mary Wheeler	Office visits, calls, E-mails	Improving performance of UTPROJ					
Jose Sanchez			Texas Victor Parr	Office visit	Training for UTPROJ and obtaining test cases					
		NPAC (S	Syracuse) - FMS & C/C							
Jeff Holland				On-site visit						
Billy Johnson		CWO			Definition of the LMS project					
Jeff Holland	CEWES	00	NPAC: Haupt		Discussion of LMS requirements					
Niki Deliman		FMS			Discussion on possible collabortion					

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT				
Niki Deliman		FMS			Definition of possible scope of the project				
Jeff Holland	CEWES	CWO		E-mail	Planning of meeting to discuss WebFlow implementation of LMS				
Billy Johnson									
Clay Lahatte		CWO		On-Site visit	Discussion and plan of				
Fred Ogden	U.Connecticut	CWO	On-Site Vi	On blee visit	implemetation of LMS				
Michael Childress	Shepherd Miller, Inc								
Niki Deliman, Burhman Gates	CEWES	FMS	EMS	EMS	NPAC: Haupt	On Site visit	Demo of mobility group application; of the scope of		
David C. Stuart	Applied Research Assocoates, Inc	LMS	Member	On-Site visit	the collaboration				
Jeff Holland									Obtaining licenses for WMS software
				CONTACT	Tutorial on how to run WMS				
Billy Johnson	CEWES	CWO			Obtaining DEM and LU data from USGS site				
I-CC II - II I				E-mails	Obtaining EDYS and CASC2D codes				
Jeff Holland							E-mails	Obtaining data sets for CASC2D	

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Jeff Holland,				E-mails	Discussions of necessary modifications to Edys and Casc2d
Billy Johnson		CWO CWO CWO		E-mails	Creating a new data sets for quick tests of Casc2d
				Visit to CEWES	First attempt to install WebFlow and web-based LMS at CEWES
Jeff Holland			NPAC: Haupt E-mail	E-mails, phone	Discussions on possible improvement of the demo
	CEWES			Visit to CEWES E-mails, phone Visit to CEWES	Improved demo of WebFlow and web-based LMS at CEWES.
Burhman Gates		MG	Member		Discussion on possibilities of collaboration
Jeff Holland		CWO		E-mails, phone	Debugging new versions of EDYS and CASC2D
				E-mails Visit to CEWES E-mails, phone Visit to CEWES	Improvement of the demo
Jeff Holland		CWO MG CWO	NPAC: Haupt	E-mails, phone	Discussion of the next steps after successful demonstration in Washington, DC

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
A CCAN III				F 7 1	Discussion of the relationship between WebFlow and WebLHA/RTI
Jeff Holland		CWO			Discussion of the new, CORBA based implementation of WebFlow
Burhman Gates	CEWES	FMS	NPAC: Haupt	Phone Calls	Redefinition of the possible scope of the collaboration
A COM III		CIVIO	-	Help with restoring the demo at CEWES	
Jeff Holland		CWO		E-mails, phone Phone Calls E-mails, phone E-mail	Providing documentation of the web-based LMS
			SPPT (Tools)		
Brian Jean	CEWES SPPT	SPPT	Rice: Breshears	Personal contact	Consulted on SPLICE (Scalable Programming Library for Coupling Executables) project
					Instructed on use of MPI_Connect software

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT		
Alan Stagg	CEWES				Consulted on SPLICE (Scalable Programming Library for Coupling Executables) project		
		SPPT			Instructed on use of TotalView debugger for ADH code on Origin2000		
Guy Robinson	Arctic Region Supercomputer Center			Personal contact	Described F90 Pthreads API and release information		
Andrew Wissink	NASA Ames Research Center				Rice: Breshears		D
Brian T. Smith	UNM, HPC Education and Research Center	CFD			Described F90 Pthreads API and release information		
Alan Wallcraft	NRL Stennis	CWO		Phone	Discuss status of support for Co-Array Fortran on CEWES machines		
Bob Robins	NRA,Inc.	CFD		Personal Contact	Discussed potential Fast Poisson solver libraries that might be able to be used at CEWES		

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Joseph Schmidt		CFD		Domest Control	Wrote, implemented and tested MPI-based code to find rank of grid edges stored across multiple processors
Zeki Demirbilek				Personal Contact	Developed algorithm to
Christine Cuicchi	CEWES	CWO	CWO		distribute CGWAVE code computations across geographically separate HPC
Trey White		CWO	Rice: Breshears	Personal Contact	Investigated current status of PTOOL Consortium projects for RF Weapons Challenge request
Trey White				Personal Contact	Investigated direct sparse solver libraries for code migration project
Matt O'Keefe	AHPCRC	CWO		Telephone	Discussed possibilities of using F90 Pthreads API in wave model code development/migration

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
Mark Fahey		SPPT			Instructed on use of TotalView debugger on CEWES IBM SP
Alex Carillo	CEWES			Personal Contact	Attempted to install requested MPI I/O package on CEWES T3E
Raju Namburu		CSM			Discussed possible SPP Tools
Fred Tracy		CFD			focused efforts to support user for upcoming year
Bob Jensen		Rice: Breshears	Personal Contact	Discussed SPP Tools support for code migration projects, specifically STWAVE and SWAN	
Ann Sherlock	CEWES	CWO		Personal Contact	Discussed SPP Tools support
Jane Smith					for code migration project, specifically STWAVE
Lori Hadley					Discussed SPP Tools support for code migration project, specifically SWAN
Shari Collela	AFRL Phillips Lab	SPPT	UTK: Browne	Phone	Browne and Collela discussed scalability problems in using Vampir with the Mach3 code that is part of the RF Weapons challenge project

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT	
James Cliburn, Hank Kuehn	CEWES			UTK: London	On-site Visit	Worked with Cliburn and Kuehn to test and install London's modified version of pbspoe on the IBM SPs so that TotalView would work correctly with parallel programs under interactive PBS
Various MSRC Users	CEWES, NAVO	SPPT	UTK: Browne	E-mail	Browne followed up on the course she taught in Dec 1998 with two email messages to class participants. The first gave an update on the SPP Tools repository and announced that TotalView was now working under interactive PBS on the IBM SPs. The second informed the class of a new web-based tutorial on Totalview.	

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	CTA	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT	
David Rhodes	Fort Monmouth, NJ	SPPT	UTK: Browne	Personal Contact, E-mail	Browne and Rhodes discussed performance issue for the CEN-1 CHSSI code the June 1998 HPCUG meeting. Rhodes was interested in trying Vampir and Browne assisted Rhode several times in using Vamp to analyze and improve the performance of his CEN-1 Harmonic Balance Simulatio code	
					Benchmarking issues relate to the IBM SP at CEWES	
Keith Bedford and David Welsh	OSU		UTK: Fagg	Visit, Phone, E-mail	Discussed MPI_Connect design and usage, assisted with MPI issues	
Andrew Wissink	NASA Ames	CWO	CWO	LVDV. D	HPC Users meeting	Dr. Wissink expressed an interest in using TotalView and Vampir on CEWES platforms.
Gerald Sasser	AFRL Phillips Lab SPPT		UTK: Browne	Phone, E-mail	Discuss continued use of Vampir with the Icepic cod inform user about SPP Too repository	

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT						
	Scientific Visualization										
Carl Cerco			NCSA: Baker, Shih	Visit, Phone, E-mail	User requirements, tool development, tool transfer						
		E014			Viualization production						
Mark Noel	CEWES Mark Noel	EQM	EQM	EQM	EQM	NCSA: Baker, Shih	Phone, E-mail	Tool development, tool transfer, and training			
			NCSA: Heiland	E-mail	Code transfer						
Robert Jensen		CWO		Visit	User requirements discussion						
Andrew Wissink	NASA Ames	CFD	NCSA: Shih	Phone, E-mail	User requirements, visualization production						
Raju Namburu		CSM			User requirepments						
D.L. (I		CWO	MSU: Machiraju		discussion and tool development						
Robert Jensen	CEWES	CWO		Visit, Phone, E-mail	Viualization production						
Mike Stephens		SV	MSU: Moorhead		Joint software development						
John West		SV		E-mail	WAM Cray-IEEE conversion						

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
			MSU: Moorhead		Discussions of WAM data formats
Mike Stephens	CEWES	SV		E-mail	Clarification of WAM data formats
			MSU: Chupa		Missing tarfile for animations
					Share our Cray binary-IEEE converter routine
Richard Allard		CWO	MSU: Moorhead		D'acces DIVA acces l'il'd'ac
Joe Metzger		CWO			Discuss DIVA capabilities
			MSU: Moorhead	Visit	ISTV development,enhancement, use
	NRLStennis		MSU: McCarter		Discussing DIVA capabilities
Peter Flynn		SV			DLT tape delivery of high-res global NLOM data
			MSU: Chupa	E-mail	ISTV 64-bit delivery
					Solaris 64-bit ISTV request

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT					
					Solaris ISTV port compilation problems					
					Solaris ISTV port gcc issues					
					Solaris ISTV port gcc issues					
					Solaris image / animation generation capability					
		nis SV MSU: Chupa		E-mail	Solaris image / animation generation capability					
	NRL Stennis S			batch-mode image generation request						
Peter Flynn			SV	SV	SV	SV	SV	MSU: Chupa		colormap generator bug fix
					global 1/32 degree data delivery					
							ISTV display gamma differences on Creator and Elite			
				Phone	ISTV display gamma differences on Creator and Elite					
					ISTV font and image saving bug report					
					ISTV ortho display request					

Table 3
CEWES USER CONTACTS

CEWES USER	USER SITE	СТА	CEWES PET Team Member	MODE CF CONTACT	PURPOSE/RESULT
					Poster image request
Peter Flynn	NRL Stennis	SV	MSU: Chupa	Phone	sun and gcc compiler problems
Robert Jensen	CWO		NOW NO 1		Set up meetings
		CWO	MSU: Moorhead	Visit	Discussions on WAM vis
Robert Jensen		CWO	MSU: Chupa	E-mail	WAM data for Hurricane Fran
Raju Namburu		CSM	MSU: Machiraju	E-mail, phone, visit	Development of project
Rama Valisetty	CEWES	CFD	USC: Prasanna, Park, Suh, Kang, Lee	E-mail	Optimized a DoD computational fluid dynamics code using the benchmarks and model developed Discussed and clarified the needs of end-users in optimizing their applications

Tool	Status	Purpose	Users	Providing Institution	Impact
			CSM		
SfcPartitioner	Under testing with CHACO	A C++ code for partitioning based on space filling curves	General use for unstructured grid partitioning to parallel processors	Texas	Moderate but broad
			SPPT		
TotalView	Purchased and installed	To provide a robust, easy-to-use tool for debugging parallel codes	Computational Migration Group (CMG) and other users that CMG supports	Tennessee	Having a single debugger that works across platforms ahs given users a higher payoff for the time investing in learning the debugger and has enabled the CMG to more effectively support users in their debugging tasks
Vampir	Purchased and installed	To provide an effective tool for analyzing and tuning communication performance of MPI parallel codes	Rhodes, White, Bova, therefore Weapons Challenge Team, Developers of MPI applications	Tennessee	Has enabled Tennessee users to quickly and easily collect performance trace data and analyze that data visually to spot communication bottlenecks in their codes.
MPI_Connect	Beta version in use by specific users, general release planned for end of March 1999	To enable interconnection and intercommunication between MPI programs running on possibly different machines with different architectures and using tuned vendor MPI implementations	Henry Gabb, Steve Bova, Clay Breshears	Tennessee	MPI_Connect enables multiple HPC systems to be used effectively on the same application, thus enabling larger problems to be solved more quickly

Tool	Status	Purpose	Users	Providing Institution	Impact
Virtue	Virtue installed on Tennessee SVC systems, vampir2virtue converter being debugged	To enable scalable visualization and analysis of large parallel applications	None yet, but targeted toward users with large-scale applications that produce large performance data trace files that cannot be visualized effectively using current tools	Tennessee, Illinois	Virtue will enable effective visualization of the execution of large-scale applications through the use of 3-D and immersive virtual reality, thus enabling performance bottlenecks to be found and fixed more easily
PAPI	Under development	To provide a portable cross-platform interface to hardware performance counters	CHSSI code and other application developers who need access to hardware performance counter data to satisfy performance reporting requirements and to tune application performance	Tennessee	The PAPI portable interface to hardware performance counters will enable users to use the same set of routines to access comparable performance data across platforms
dyninst	Tested on Tennessee IBM SP2, being tested on CEWES MSRC IBM SP pandion, being ported by University of Wisconsin to SGI/Cray Origin 2000	To enable users to dynamically insert and remove instrumentation into and from a running application	None yet, but aimed at sophisticated users willing to learn a low-level but powerful interface for runtime application instrumentation	Maryland, Tennessee	dyninst will enables users to attach to a running application and monitor or even change application behavior dynamically

Tool	Status	Purpose	Users	Providing Institution	Impact
DPCL	Awaiting installation on IBM SP pandion, being ported to SGI/Cray Origin 2000	To provide a higher-level client-server interface to dyninst for use in parallel and distributed environments	None yet, but aimed at users who need to be able to dynamically attatch to a running parallel or distributed application and monitor or change application behavior at runtime	Tennessee (IBM)	DPCL will provide a cross-platform infrastructure for runtime application instrumentation for the purposes of performance analysis, computational steering, and data visualization
Repository in a Box (RIB)	Tennessee RIB repositories currently hosted at Tennessee. RIB released and available for installation at Tennessee	To facilitate setting up and maintaining an interoperable and distributed collection of software repositories for CTAs and PET support areas	All	Tennessee	RIB provides an easy-to-use interface for CTA onsite leads to enter and maintain information about software being made available to MSRC users as a result of PET and CHSSI efforts
Fortran 90 Pthreads API	Coding is complete; testing and documentation are near completion; awaiting CEWES MSRC Government approval for public release	Provide access to POSIX threads functionality within Fortran codes	All	Rice, MSU, NRC	Pthreads is a concurrent model for shared-memory programming. It has a simple, portable interface with powerful functionality that allows MSRC users a relatively quick migration path for their serial or vector codes to parallel machines

Tool	Status	Purpose	Users	Providing Institution	Impact					
	C/C									
Tango Interactive	Installed at CEWES MSRC, JSU, MSU, CAU	Distance education and training, remote collaboration	All interested in remote collaboration and training	Syracuse University	Used to deliver academic credit classes to JSU, CEWES MSRC, and elsewhere; used to deliver two prototype distance trainings, the larger of which encompassed all four MSRCs, NRL-DC, and the Ohio Supercomputer Center.					
			SV							
CbayVisGen	Installed	Visualization	Cerco, others	NCSA	Enables vis of long-duration runs of CE-QUAL-IQM					
Transport Flux Vis	First release installed	Visualization	Cerco, others	NCSA	Enables vis of transport flux data from CE-QUAL-IQM					
NCSA vss 3.0	Delivered	Data Sonification	Potentially all	NCSA	Enables use of sound in data analysis					
NCSA ViaVoice Speech Support	Delivered	Speech interfaces	Potentially all	NCSA	Enables natural user interfaces					
FLTK	Advised use	GUI building	Potentially all	NCSA	Supports fast building of graphical user interfaces					

Tool	Status	Purpose	Users	Providing Institution	Impact
ISTV	Installed CEWES ITL, NAVO VisLab, and NRL/SSC	CWO/EQM/CFD visualization	CWO model users (Wornom, Welsh) and SV personnel at CEWES, NRL/SSC NLOM modelers and analysts (Flynn), NAVO/MSRC vislab personnel (Gruzinskas)	MSU	Allows interactive visualization of high-resolution models on desktop workstations, has distributed reader so less computation must be done on local workstation, allows CWO/EQM/CFD visualization on Sun workstations

This page intentionally left blank

Code	Nature of Code	CEWES MSRC User(s)	Institutions Involved	Result	
CRAFT		Don Kenzakowski and others	MSU, NRC, CRAFT Inc	Work in progress	
HELIX	CFD Solver	Marty Moulton and others	MSU, Rice, NRC, NASA Ames	Code optimized, attempt to parallelize with OpenMP in progress by Rice	
MICOM	CWO solver	Matt O'Keefe	MSU, NRC, NRL, University of Minnesota	Improvements in portability considered via Pthreads	
IFLOW	CFD Solver	Chao-Ho Sung	MSU, NRC, NRL	Referred to parallel multigrid solver from MGNET or switch to CHSSI code	
a.out	CCM Solver	Stephen Hellberg	MSU, NRC, NRL	Work in progress. Code validation to be automated using nonlinear optimization strategies	
CGWAVE		Zeki Demirbilek	MSU, NRC, CEWES	Parallelized for all platforms using MPI, for SGI using Dual-level MPI and OpenMP, and for all shared-memory systems using OpenMP	
NSTURB3D	CWO solver	Fernando Grinstein	CEWES MSRC, MSU, NRL	Work in progress. Parallelization underway using MPI	
CH3D-SED		Billy Johnson	MSU,OSU	MPI parallel implementation of non-cohesive sediment version	
HIVEL2D		Charlie Berger	MSU	Demonstrated and publicized computational design capability	
СТН	CSM (penetration, impact and strong shock analysis)	Raju Namburu	Texas	Provide error indicators and adaptive capability in parallel CTH	
EPIC	CSM (impact and penetration analysis)	Mark Adley	Texas	Prototype local adaptive capability and error indicators added to EPIC	

Code	Nature of Code	CEWES MSRC User(s)	Institutions Involved	Result
CH3D	CWO marine circulation model	Billy Johnson	Ohio, CEWES	Coupled with WAM at atmospheric boundary layer using MPI
CH3D-SED	CWO marine circulation mode	Billy Johnson	Ohio, MSU, CEWES	Parallelized for O2K and T3E using MPI
WAM	CWO wind-wave model	Bob Jensen	Ohio, CEWES	Coupled with CH3D at atmospheric boundary layer using MPI; parallelized for O2K using OpenMP; corrected sign errors in propagation scheme; modified bottom friction algorithm to account for currents
SWAN	CWO wind-wave model	Lori Hadley	Ohio, CEWES, Rice, NRC, CEWES MSRC CMG	Currently working on parallelization on O2K using OpenMP
FEMWATER	Groundwater flow	Jeff Holland, Fred Tracy	Texas, CEWES	Parallelized for T3E using MPI
CE-QUAL-ICM	Water-quality	Mark Dortch, Carl Cerco, Barry Bunch, Mark Noel	Texas, CEWES	Parallelized for SGI O2K, Cray T3E, and IBM SP using MPI
CE-QUAL-ICM/T OXI	Water-quality	Mark Dortch, Barry Bunch, Terry Gerald	Texas, CEWES	Parallelized for SGI O2K using MPI
ADCIRC	Hydrodynamics	Rao Vemulakunda, Joannes Westerink, Rick Luettich	Texas, CEWES, Notre Dame, UNC	Parallelized for SGI O2K, Cray T3E, and IBM SP using MPI
MAGI	Smoothed Particle Hydrodynamics code	David Medina	Rice	Factor of two improvements on O2K by data and computation reordering
HELIX	CFD code for computing transonic flow on a rotor	Marvin Moulton	Rice	4 to 12% improvements in performance on SGI O2K, Cray T3E and IBM SP2 by scalar replacement

Code	Nature of Code	CEWES MSRC User(s)	Institutions Involved	Result
CEN-1, Harmonic Balance Simulation	CEN CHSSI code	David Rhodes	Tennessee	By using Vampir to view performance data obtained using Vampirtrace, which had very low intrusion, David Rhodes was able to determine how to make significant algorithmic changes in his task scheduling approach that achieved much better levels of scalability and parallel efficiency for the CEN-1 CHSSI code
CGWAVE	Large-scale oceanographic simulation	Henry Gabb, Steve Bova, Clay Breshears	CEWES and ASC MSRCs, Tennessee	CGWAVE is used daily by the Navy for forecasting and analysis of harbor conditions. By using a combination of OpenMP, MPI, and MPI_Connect to run CGWAVE with multiple levels of parallelism across Origin 2000s at CEWES and ASC MSRCs, the CEWES MSRC team was able to reduce the runtime from over 6 months to less than 72 hours for modeling wave motions in Ponce Inlet off the Florida coast. This project won the Most Effective Engineering Methodology award for the HPC challenge at SC98
Icepic	Part of Radio-Frequency Weapons DoD Challenge project	Gerald Sasser	Tennessee	By using Vampir to view performance data obtained using Vampirtrace, including making calls to the Vampirtrace API to relate performance data to the source code, Gerald Sasser was able to identify portions of the Icepic code where communication bottlenecks were occurring. Changes to the way the communication was implemented resulted in 33% speedup of that part of the code

Code	Nature of Code	CEWES MSRC User(s)	Institutions Involved	Result
MSPHERE	CWO	Steve Slinker	CEWES MSRC CMG, Tennessee	In a recent migration project (a code called MSPHERE), TotalView was used to isolate a Cray pointer bug on the SGI O2K. The ported code gave incorrect results regardless of compiler options. The code made extensive use of Cray pointers, and often passed them as arguments. However, the receiving dummy arguments were sometimes integers. When the receiving integer was not large enough to hold a memory address, the program produced incorrect results. This type of bug would have been very difficult to find without TotalView
CE-QUAL-IQM	EQM/Vis	Cerco, others	NCSA	Instrumented parallel version of CE-QUAL-IQM for use with CUMULVS, pV3, DICE ISTV, SV, SV and CWO modelers, MSU, Port to Solaris 32-bit for modelers' desktop machines. ISTV, SV, SV and CWO modelers, MSU, Port to IRIX 64-bit so that large WAM and NLOM files (~6GB) can be visualized interactively. ISTV, SV, SV and CWO modelers, MSU, Port to Solaris 64-bit to provide similar functionality for Suns ISTV, SV, SV and CWO modelers, MSU, WAM reader utilities

Code	Nature of Code	CEWES MSRC User(s)	Institutions Involved	Result
FLOW	DoD CFD application	Rama Valisetty	USC, CEWES MSRC	Optimized the previous implementation 5 fold when using 30 processors. An optimal partitioning and mapping of the data cube and processors achieved good load balancing with minimal communication cost. Parallel communication and latency hiding techniques dramatically reduced the interprocessor communication cost for the parallelized algorithm
DYNA3D, INGRID and ParaDyne	CSM Code	Dr. Raju Namburu	CAU	Bi-Directional Data Translation on the SGI, Power Challenge and IBM SP. NOTE: Awaiting Parallel version of DYNA3D

This page intentionally left blank

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
Dual-Level Parallel Algorithms using MPI and OpenMP	PET Technical Reportt, presentations	MSU, Rice, NRC	To exploit next generation of HPC systems with distributed clusters of shared-memory processors Zeki Demirbilek of CEWES		Any user who has an MPI code could potentially benefit by adding OpenMP parallelism as well, particularly those who are exploring a linear parameter space
Significant reduction in turnaround time enabling larger scale simulations	Parallel Programming Expertise, Technical Reports, Short courses	MSU, Rice, NRC	To assist MSRC users to choose an appropriate parallel programming model (e.g. MPI, HPF, OpenMP) when parallelizing their code	David Medina, AFRL Phillips Lab	Potentially all users of parallel MSRC computers. The MSRC will benefit if its machines are used in a more efficient way due to knowledgeable users
Block Adaptive Parallel CTH	IAT/Texas & SNLA	Texas	To extend the CTH capability to parallel adaptive simulation	Raju Namburu, Kent Kimsey, Dan Scheffler, David Kleponis	More reliable results and more efficient
Local Adaptive EPIC	G. Johnson (Alliant Techsystems Inc.) and Texas	Texas	To extend EPIC for adaptive unstructured refinement with appropriate error indicators	Mark Adley, Steve Akers CEWES , Kirk Vanden (Eglin AFB)	These are the very first calculations of this type, impact potential is very high
Parallelization Methodology	EQM team at Texas	Texas	Parallelize large class of EQM codes	Mark Dortch, Carl Cerco, rallelize large class of Mark Noel, Barry Bunch,	

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
Grid Partition Software	AHPCRC, University of Minnesota	Texas	Improve parallel performance of EQM codes Mark Dortch, Carl Cerco, Mark Noel, Barry Bunch, Rao Vemulokanda, Terry Gerald, Fred Tracy		FEMWATER, CE-QUAL-ICM, CE-QUAL-ICM/TOXI, ADCIRC
CAPTools communication library on T3E	University of Greenwich	Rice	To be able to run codes parallelized by CAPTools All parallel code developer using CAPTools		Support CAPLIB library
Dynamic Instrumentation	University of Wisconsin, University of Maryland, IBM	(Tennessee	To enable users to attach to a running application and dynamically monitor, analyze, steer the computation	Developers of large, long-running applications	Dynamic instrumentation techniques overcome the limitations of trace-based techniques by eliminating the need to save and analyze large unwieldy trace files and by allowing interactive real-time monitoring and steering of applications
Debugging and performance analysis tools	Various vendors and research groups	Tennessee	To provide tools for effective debugging and performance analysis of parallel applications	All	The SPP Tools repository at provides an up-to-date listing of debugging and performance analysis tools available on CEWES MSRC platforms. A concise matrix view provides an at-a-glance summary of what tools are available on what platforms, as well as links to site-specific usage information and tutorials

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
Access to hardware performance counters	Various vendors	Tennessee	To provide a portable interface to hardware performance counters available on MSRC platforms	CHSSI code developers and other MSRC users who need access to hardware performance counter data for meeting performance reporting requirements and for tuning application performance	The portable interface to hardware performance counters being developed by Tennessee will enable MSRC application developers to use the same set of routines to access comparable performance counter data across platforms
WebFlow distributed computing environment	Syracuse	Syracuse	Facilitate use of distributed HPC resources by applications developers and by users based on standard and commodity technologies	Land Management System (Jeff Holland), Mobility Systems Group (Niki Deliman). Potentially all CTAs	Provides the ability to provide web-based user interfaces to HPC applications and to simplify application usage of HPC resources
Data management	NCSA	NCSA	Data storage and access	Potentially all	Better data management
dlMedia library image and movie capture	NCSA	NCSA	Easy image and movie capture	Cerco	Asynchronous vis collaboration
Transport flux vis	NCSA	NCSA	Transport flux visualization	Cerco	New vis capability
Computational monitoring software	ORNL	NCSA	Visualization of running code	Potentially all	Dynamic vis capability
Collaborative visualization	NCSA	NCSA	Collaborative visual analysis of simulation output	Cerco	Synchronous vis collaboration

Technology	Source	Providing Institution	Purpose	CEWES MSRC Users	Impact
User interface building software	EasySW	NCSA	GUI building	Stephens	Faster tool development
Speech input IBM	NCSA	NCSA	Speech input into virtual reality applications	Stephens	Natural user interfaces
Non-speech audio output	NCSA	NCSA	Using audio for sonfication and data analysis	Stephens	New data analysis capability
Wavelet encoding	MSU	MSU	Feature-based encoding	Namburu	Better data storage and vis
ISTV	MSU	MSU	Visualization	Jensen, Wallcraft	New vis capability
High-resolution visualization	MSU	MSU	Vis package with efficient storage architecture	CWO specifically—others as well	Allows use of modest desktops to examine large-scale data interactively
Wavelet algorithms, volume rendering algorithms	MSU	MSU	Allow better understanding of datasets	Namburu	Allows access to useful tools enabling CSM users to visualize data easily; such tools did not exist
USC Benchmarks and IMH Model	USC	USC	Performance modeling and optimization of user code on parallel machines	Application developers on IBM SP, SGI/Cray T3E, and SGI/Cray O2K	Efficient scalable and portable code migration

Table 7 TRAINING COURSES

Course Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees	Rating		
Note: Attendees broken down by: (on-site MSRC users, off-site MSRC users, PET/integrator personnel, HBCU/MI personnel, other)									
Using the Message-Passing Interface (MPI)	NRL	4/29-5/1/98	MSU	Puri Bangalore and Shane Hebert	Lecture and labs	5(0,5,0,0,0)	5.0		
Large Deformation Computational Structural Mechanics, Applications on High Performance Computers using ParaDyn/DYNA3D	CEWES MSRC	5/5-5/6/98	LLNL	Jerry Lin and Carol Hoover	Lecture, demonstration and hands-on training	10(7,3,0,0,0)	N/A		
Grid Generation for Complex Configurations		5/12-5/13/98	MSU	Bharat Soni, Brian Jean, Tim Tautges, Shayar Pirzadeh, Rick Weed	Lecture, demonstation and hands-on exercises, MBONE	10(4,3,2,0,1)	3.8		
Java for Scientific Computing		5/19-5/21/98	Syracuse	Nancy McCracken	Lecture and labs, MBONE	10(9,0,1,0,0)	4.5		
Grid Generation for Complex Configurations		6/1/98	MSU	Hugh Thornburg, Ray Gomez	Lecture and labs	10(0,7,2,0,1)	N/A		
Using the Message-Passing Interface (MPI)	DoD HPCMP Users	6/1/98	MSU	Puri Bangalore	Lecture	22(2,10,2,3,5)	N/A		
High Performance Fortran	Group	6/1/98	Rice	Charles Koelbel	Lecture	12(1,7,0,0,4)	N/A		
Performance Optimization	Meeting at Rice	6/1/98	Tennessee	Phil Mucci, Kevin London	Lecture and labs	20(0,15,1,0,4)	N/A		
Topics in Finite Element Methodology		6/1/98	Texas	Graham Carey	Lecture	15(1,7,4,0,3)	N/A		

Table 7 TRAINING COURSES

Course Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees	Rating
Using the Message-Passing Interface (MPI)	CEWES	6/17-6/19/98	MSU	Puri Bangalore and Shane Hebert	Lecture and labs	3(1,1,1,0,0)	5.0
Parallel Programming Workshop for Fortran Programmers	MSRC	6/22-6/26/98	CEWES MSRC, MSU	Dan Nagle, Rick Weed	Hands-on labs	3(2,1,0,0,0)	4.7
A Tutorial on Designing and Building Parallel Programs	NRL	8/3-8/4/98	Rice	Gina Goff, Ehtesham Hayder, Charles Koelbel	Lecture and labs	3(0,3,0,0,0)	5.0
A Tutorial on Designing and Building Parallel Programs		8/6-8/7/98	Rice	Gina Goff, Ehtesham Hayder, Charles Koelbel	Lecture and labs	6(4,0,2,0,0)	4.0
An Introduction to Fortran 90		9/28/98	Ohio Supercomputer Center	Troy Baer	Lecture, Tango	14(9,1,4,0,0)	4.2
Scalable OpenMP programming on Origin2000	CEWES	10/21/98	Silicon Graphics	Ramesh Menon	Lecture	13(3,0,6,0,4)	4.8
Introduction To MSC/PATRAN - Modeling for Design Analysis	MSRC	10/28-10/30/9	MacNeal Schwendler Corp	Bart McPheeters	Lecture and hands-on labs	8(6,1,1,0,0)	4.5
Parallel Programming Workshop for Fortran Programmers		11/9-11/13/98	CEWES MSRC, MSU	Dan Nagle , Rick Weed	Hands-on labs	4(0,2,1,0,1)	4.8
Tango for Remote Consulting		11/17-18/98	Syracuse	Marek Podgorny, Scott Klasky, Remek Trzaska	Lecture and labs, MBONE	5(2,0,3,0,0)	4.8

Table 7 TRAINING COURSES

Course Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees	Rating
Parallel Programming Workshop for Fortran Programmers	Electric Boat Co.	12/7-12/11/98	CEWES MSRC, MSU	Dan Nagle and Rick Weed	Hands-on labs	10(0,10,0,0,0)	N/A
Parallel Debugging and Performance Analysis Tools: TotalView and Vampir		12/8-12/9/98	Tennessee	Shirley Browne	Lecture and hands-on exercises	9(3,1,5,0,0)	4.2
Techniques in Code Parllelization		1/7-1/8/99	Texas	Mary Wheeler, Clint Dawson, Victor Parr	Lecture	10(5,2,2,0,1)	2.5
Parallel Programming on the Origin2000 using OpenMP	CEWES MSRC	1/26-1/27/99	Ohio Supercomputer Center	David Ennis	Lecture and labs, Tango	24(5,11,7,0,1)	4.4
Computational Monitoring Using CUMULVS		1/28/99	NCSA	Dave Semeraro, Randy Heiland	Lecture and labs	6(4,0,2,0,0)	4.0
Interactive Structured Time-varying Visualizer (ISTV)		1/29/99	MSU	Michael Chupa, Robert Moorhead	Lecture and labs	5(2,1,3,0,0)	4.0
WebFlow: Web Interfaces for Computational Modules		3/9/99	Syracuse	Tomasz Haupt	Lecture and labs	14(11,0,2,0,1)	3.8

This page intentionally left blank

Table 8 TRAINING COURSES & SEMINARS at HBCU/MIs

Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees *	
* Number of attendees broken down by: (Undergraduates, Graduate Students, Faculty/Staff)							
Spring 1999							
CSC539 Advanced Web Programming	JSU	16 Weeks	Syracuse	Dr. McCracken	Web-Based using Tango	8 (0,8, 0)	
CSC499 Programming for the Web	Morgan State University	16 Weeks	JSU	Dr. Malluhi	Web-Based using Tango	5 (5, 0, 0)	
CSC539 Advanced Web Programming	Clark-Atlanta	16 Weeks	Syracuse	Dr. McCracken	Web-Based using Tango	4 (0, 4, 0)	
Fall 1998							
CSC539 Computational Science for Simulation Application	JSU	16 Weeks	Syracuse	Dr. McCracken	Web-Based using Tango	8 (0,8, 0)	
Spring 1998							
CSC499 Programming for the Web	JSU	16 Weeks	Syracuse	Dr. McCracken	Web-Based using Tango	9 (8, 0, 1)	
JSU HPC Summer Institute							
High Performance Computing Overview	JSU	1 day	CEWES MSRC	Dr. Louis Turcotte	Lecture	20 (20, 0, 0)	

Table 8
TRAINING COURSES & SEMINARS at HBCU/MIs

Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees *
Environmental Quality Management (EQM)	JSU	1 day	Texas	Prof. Mary Wheeler, Dr. Bob Fithen, Dr. Monica Martinez-Carales	Lecture	20 (20, 0, 0)
Environmental Quality Management (EQM) Lab	JSU	1 day	Texas	Sharon Lozano	Lab	20 (20, 0, 0)
Computational Structural Mechanics (CSM)	JSU	1 day	NCSA	LaRay Dandy	Lecture	20 (20, 0, 0)
Computational Structural Mechanics (CSM) Lab	JSU	1 day	MSU	Dr. Richard Weed	Lab	20 (20, 0, 0)
Climate/Weather/Ocean Modeling and Simulation (CWO)	JSU	1 day	osu	Prof. Keith Bedford, Prof. Ponnuswamy Sadayappan	Lecture	20 (20, 0, 0)
Climate/Weather/Ocean Modeling and Simulation (CWO) Lab	JSU	1 day	osu	Dr. David Welsh, Prof. P. Sadayappan, Shuzia Zhang	Lab	20 (20, 0, 0)
Computational Fluid Dynamics (CFD)	JSU	1 day	MSU	Prof. Jan-Ping Zhu	Lecture	20 (20, 0, 0)
Computational Fluid Dynamics (CFD) Lab	JSU	1 day	MSU	Dr. Steven W. Bova	Lab	20 (20, 0, 0)
Forces Modeling and Simulation (FMS)	JSU	1 day	Syracuse	Dr. Wojek Furmanski, Tom Pulikal, Subhah Nair	Lecture	20 (20, 0, 0)

Table 8 TRAINING COURSES & SEMINARS at HBCU/MIs

Title	Location	Duration	Providing Institution	Instructor(s)	Format	Number of Attendees *
Forces Modeling and Simulation (FMS) Lab	JSU	1 day	Syracuse	Dr. Wojek Furmanski	Lab	20 (20, 0, 0)
Scalable Parallel Programming Tools (Tools)	JSU	1 day	Rice	Dr. Charle Koelbel	Lecture	20 (20, 0, 0)
Scalable Parallel Programming Tools (Tools) Lab	JSU	1 day	Rice	Dr. Cay P. Breshears	Lab	20 (20, 0, 0)
Scientific Visualization (Sci Viz)	JSU	1 day	NCSA	Dr. Alan Shih	Lecture	20 (20, 0, 0)
Scientific Visualization Lab	JSU	1 day	NRC	Dr. Richard Strelitiz	Lab	20 (20, 0, 0)
Computer Graphics and Animation	JSU	1 day	JSU	Edgar Powell, Milti Leonard	Lecture, Lab	20 (20, 0, 0)

This page intentionally left blank

Student	Level	Major	University	Impact
ICH HDC C I. 224	4- C4 I4-			
JSU HPC Summer Instit	ute Students			
Aldrice Bell	Freshman	Electric Engineering	Florida A&M	
Andrea Carter	Sophomore		Alcorn State University	
Onekki Christian	Freshman		T. 1. G. (11)	
Taheerah Fulgha		Computer Science	Jackson State University	
Ebony Gaston	Sophomore			
Aisha Gates	237	Computer Science/Applied Math	Alcorn State University	
Terri Lynn Grant	Freshman	Labora State University	Jackson State University	
Aarion Gray	Sophomore	Computer Science		
Ollie Hales	Freshman		Dillard University	Summer Institute 1998
Stephanie Hall	Junior	Biology/Pre-med	Jackson State University	
Tammy Harris	Junior	Mat /Communication	Tougaloo College	
Kenneth Jackson	Freshman	Math/Computer Science	Alcorn State University	
Wayne Jackson	Junior			
Sharon James	Sophomore	Computer Science	Jackson State University	
Joyce Mayfield	Junior		Alcorn State University	
Abdul Mohammed	Freshman	Math/Pre-Engineering		
Kimberly Neal	Junior	Computer Science	Jackson State University	

HBCU/MI STUDENTS IMPACTED						
Student	Level	Major	University	Impact		
Kiana Randle	Sophomore	Mathematics	Alcorn State University	G I 1000		
Jennifer Rawls	Graduate	Computer Science	Jackson State University	Summer Institute 1998		
Distance Learning Cours	ses (Spring 1998) CSC499	Programming for the W	/eb			
Angela D. Robinson						
Dionte S. Wilson						
Douglas W. Holton			Jackson State University			
Gloria A. Davenport		Computer Science		D		
John H. Young	Junior			Distance Learning Course		
Krystal S. Cooper						
Marvin A. Winfield						
Marvin A. Winfield						
Distance Learning Cours	ses (Fall 1998) CSC539 Co	omputational Science for	Simulation Applications			
Brittian, Wendy Faye						
Chava, Srinivasa Rao						
Jin, Lingyun	Graduate	Computer Science	Jackson State University	Distance Learning Course		
Kureishi, Tushar		r		6		
Madubanya, Matsobane						

Martin

HBCU/MI STUDENTS IMPACTED							
Student	Level	Major	University	Impact			
Safaya, Usha							
Hemant Mahidhara				D			
Zheng, Shenyu	Graduate	Computer Science	Jackson State University	Distance Learning Course			
Dabade, Ajit Kamalakar							
CSC499 Programming for	r the Web (Spring 1999)						
Dawn Ambrose							
Annette Harris							
Cynthia Ann Gibson	Junior		Morgan State University				
Robin Tucker							
Danny McLellan							
Robert Thomas							
Jiao Hengli		Computer Science		Distance Learning Course			
Roy Harrington							
Rashad Evans							

Jackson State University

Kirk Williams

Quinn McGill

Veronica Johnson

Dennis Thompson

Senior

Student	Level	Major	University	Impact
Monica Harris	Senior	Computer Science	Jackson State University	Distance Learning Course
Sharice McElroy				
Tamara Jones				
Latonia Logan				

CSC539 Advanced Web Programming (Spring 1999)

Aalati, Vijaya Kumar Reddy				
Bhagwat, Dinesh R				
Chilka, Anoop Kumar				
Dogiparthy, Sreedhar				
Madubanya, Martin Matsobane			Jackson State University	
Mahidhara, Hemant M				
Reddy, Satish Reddy	Graduate	Computer Science		Distance Learning Course
Sridhar, Aswatha				
Naidu, Shilpa S, P				
Shilpa Jahagirdar				
Pradeep Jandepaneni			Cl. 1 Ad	
Jammie Lockett			Clark-Atlanta	
Kennard Love				

Presenters	Торіс	Place	Date					
	CFD, CWO							
P. Bangalore, J. Zhu, D. H. Huddleston, A. Skjellum, D. J. Welsh and R. Wang	"Parallelization of a Hydraulics and Sediment Transport Simulation Code"	DoD HPCMP Users Group Conference, Monterey CA	June 1999					
	CFD, SPPT							
S. W. Bova, C. P. Breshears, H. A. Gabb, C. Cuicchi, and Z. Demirbilek	"Dual-Level Parallel Analysis of Harbor Wave Response using MPI and OpenMP"	HPC Challenge Demo Competition, SC98, Orlando FL	November 1998					
S. W. Bova, C. P. Breshears, C. Cuicchi, Z. Demirbilek, and H. A. Gabb	"Dual-Level Parallel Analysis of Harbor Wave Response using MPI and OpenMP"	Submitted to: International Journal of High Performance Computing Applications	1999					
S. W. Bova, C. P. Breshears, C. Cuicchi, Z. Demirbilek, and H. A. Gabb	"Nesting OpenMP in an MPI Application"	Submitted to: PDCS-99, 12th International Conference on Parallel and Distributed Computing Systems, Ft. Lauderdale FL	1999					
S. W. Bova, C. P. Breshears, C. Cuicchi, Z. Demirbilek, and H. A. Gabb	"Using MPI_Connect to Distribute Parallel Applications Across Multiple Platforms"	Submitted to 1999 International Conference on Parallel and Distributed Processing Techniques and Applications, Las Vegas NV	1999					
S. W. Bova, C. P. Breshears, H. A. Gabb, R. Eigenann, G. Gaertner, R. Kuhn, W. Magro, S. Salvini	"Parallel Programming with Message Passing and Directives"	Invited review, SIAM News, in press, 1999	1999					

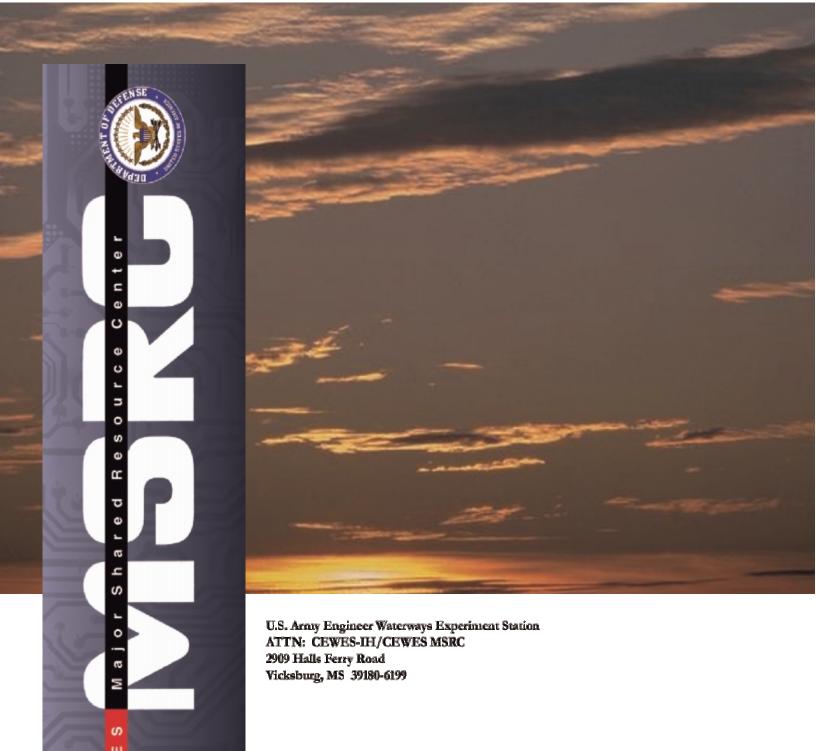
Presenters	Topic	Place	Date
S. W. Bova, C. P. Breshears, C. Cuicchi, Z. Demirbilek and H. A. Gabb	"Nesting OpenMP in an MPI Application"	Submitted to 11th International Conference on Parallel and Distributed Computing and Systems	1999
C. P. Breshears and G. Fagg	"A Computation Allocation Model for Distributed Computing Under MPI_Connect"	1st Southern Conference on Computing, Hattiesburg MS	1999
C. P. Breshears, S. W. Bova, C. Cuicchi, Z. Demirbilek and H. A. Gabb	"Using MPI_Connect to Distribute Parallel Applications Across Multiple Platforms"	Submitted to The 1999 International Conference On Parallel And Distributed Processing Techniques And Applications	1999
C. P. Breshears, H. A. Gabb and S. W. Bova	"Towards a Fortran 90 Interface to the POSIX Threads Library"	DOD HPC Users Group Meeting, Houston TX	June 1998
H. A. Gabb, R. P. Bording, S. W. Bova and C. P. Breshears	"A Fortran 90 Application Programming Interface to the POSIX Threads Library"	40th Cray UserGroup Conference, Stuttgart, Germany	June 1998
H. Gabb, P. Bording, S. W. Bova, C. P. Breshears and D. Medina	"Expressing Fine-Grained Parallelism Using Fortran Bindings to Posix Threads"	40th Cray User Group Conference, Stuttgart, Germany	June 1998
	SPPT		
M. Browne	"Software Deployment Grid Article from LINK",	ARL MSRC Newsletter	Fall 1998
S. Browne, J. Dongarra, J. Horner, P. McMahan, and S. Wells	"The National HPCC Software Exchange (NHSE): Uniting the High Performance Computing and Communications Community"	DLIB Magazine	May 1998
S. Browne and C. P. Breshears	"Usability Study of Portable Parallel Performance Tools"	DoD HPCMP Users Group Meeting, Houston TX	June 1998

Presenters	Topic	Place	Date	
M. E. Hayder and J. Mellor-Crummey	"Improving Performance by Scalar Replacements"	DoD Users Group Conference, Monterey CA	June 1999	
B. Jean, A. Stagg and C. P. Breshears	"A Scalable Programming Library for Coupling Executables (SPLICE)"	Poster at SC98, Orlando FL	November 1998	
H. Park, D. Kang, J. Suh, and V. Prasanna	"Benchmarking and Modeling of High Performance Computing Platforms"	DoD HPCMP Users Group Conference, Monterey CA	June 1999	
	EQM			
S. Chippada, C. Dawson, V. Parr, M. F. Wheeler, C. Cerco, B. Bunch and M. Noel	"PCE-QUAL-ICM: A Parallel Water Quality Model Based on CE-QUAL-ICM"	DOD HPC Users Group Meeting, Houston TX	June 1998	
SV				
M. A. Chupa, R. J. Moorhead II, S. Nations, A. Johannsen, K. Gaither, and R. Vickery	"ISTV: Interactive Structured Time-varying Visualizer"	Submitted to IEEE Oceans'99	1999	
FMS				
D. Bernholdt, P. Chappell, G. C. Fox, W. Furmanski, D. Kasthuril, G.Krishnamurthy, S. Nair, H. T. Ozdemir, Z. Odcikin-Ozdemir, K. Rangarajan and K. Snively	"Parallel and Metacomputing Support for CMS – Comprehensive Minefield Simulation"	SC98, Orlando FL	November 1998	
D. Bernholdt, G. C. Fox, W. Furmanski, B. Natarajan, H. T. Ozdemir, Z. Odcikin-Ozdemir and T. A. Pulikal	"WebHLA - An Interactive Programming and Training Environment for High Performance Modeling and Simulation"	SC98, Orlando FL	November 1998	

Presenters	Topic	Place	Date
G. C. Fox, W. Furmanski, G. Krishnamurthy, H. T. Ozdemir, Z. Odcikin-Ozdemir, T. A. Pulikal, K. Rangarajan and A. Sood	"Using WebHLA to Integrate HPC FMS Modules with Web/Commodity based Distributed Object Technologies of CORBA, Java, COM and XML"	Advanced Simulation Technologies Conference (ASTC99), San Diego CA	April 1999
G. C. Fox, W. Furmanski, S. Nair, H. T. Ozdemir, Z. Odcikin-Ozdemir and T. A. Pulikal	"WebHLA - An Interactive Multiplayer Environment for High Performance Distributed Modeling and Simulation"	International Comference on Web-based Modeling and Simulation, WebSim99, San Francisco CA	January 1999
G. C. Fox, W. Furmanski, H. T. Ozdemir and S. Pallickara	"New Systems Technologies and Software Products for HPCC: Volume II - High Performance Commodity Computing on the Pragmatic Object Web"	for RCI, Ltd	October 1998
G. C. Fox, W. Furmanski, S. Nair, H. T. Ozdemir, Z. Odcikin-Ozdemir and T. A. Pulikal	"WebHLA - An Interactive Programming and Training Environment for High Performance Modeling and Simulation"	SISO Simulation Interoperability Workshop, SIW Fall 98, paper SIW-98F-216, Orlando FL	September 1998
G. C. Fox, W. Furmanski, B. Goveas, B. Natarajan and S. Shanbhag	"WebFlow-Based Visual Authoring Tools for HLA Applications"	International Test and Evaluation (ITEA) Workshop on High Performance Computing, Aberdeen MD	July 1998
G. C. Fox, W. Furmanski, S. Nair and Z. Odcikin-Ozdemir	"Microsoft DirectPlay meets DMSO RTI for Virtual Prototyping in HPC T&E Environments"	International Test and Evaluation (ITEA) Workshop on High Performance Computing, Aberdeen MD	July 1998
G. C. Fox, W. Furmanski and H. T. Ozdemir	"Object Web (Java / CORBA) based RTI to Support Metacomputing M&S"	International Test and Evaluation (ITEA) Workshop on High Performance Computing, Aberdeen MD	July 1998

Presenters	Topic	Place	Date
G. C. Fox, W. Furmanski and T. A. Pulikal	"Evaluating New Transparent Persistency Commodity Models: JDBC, CORBA PSS, OLEDB and W3C WOM for HPC T&E Databases"	International Test and Evaluation (ITEA) Workshop on High Performance Computing, Aberdeen MD	July 1998
G. C. Fox, W. Furmanski and H. T. Ozdemir	"Java/CORBA based Real-Time Infrastructure to Integrate Event-Driven Simulations"	Collaboration and Distributed Object / Componentware Computing, PDPTA 98, Las Vegas NV	July 1998
	CFD		
D. H. Huddleston , R. C. Berger and C. Berg	"A Numerical Design Method for Open-Channel Flow"	1998 ASCE International Water Resources Engineering Conference, Memphis TN	August 1998
J. White and S. W. Bova	"Portability Issues Associated with Overlapping MPI Communication and Computation"	Poster presentation SC98, Orlando FL	November 1998
J. White and S. W. Bova	"Issues Concerning Overlapping MPI Communication with Computation for Parallel Krylov Methods"	Mini symposium lecture, 5th SIAM Conference on Mathematical and Computational Issues in the Geosciences, San Antonio TX	1999
J. White and S. W. Bova	"Where's the Overlap? An Analysis of Popular MPI Implementations"	MPIDC, Atlanta GA	1999
J. Zhu, B. Johnson, P. Bangalore, D. H. Huddleston and A. Skjellum	"On the Development of A Parallel Three-Dimensional Hydrodynamic Simulator"	1998 ASCE International Water Resources Engineering Conference, Memphis TN	August 1998

Presenters	Topic	Place	Date		
CSM					
A. Patra and D. Littlefield	"A report on Error Indicators for Lagrangian ImpactMechanics Codes"	Institute for Advanced Technology Technical Report No. IAT.R, University of Texas	In publication, 1999		
CWO					
D. J. S. Welsh, R. Wang, P. Sadayappan, and K. W. Bedford	"Coupling of Marine Circulation and Wind-Wave Models on Parallel Platforms"	DoD HPCMP Users Group Conference, Monterey CA	June 1999		



For further information, contact:

CEW

CEWES MSRC

Customer Assistance Center Web site http://wes.hpc.mil Email at info-hp@wes.hpc.mil Telephone at 800-500-4722